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IP1

Opening Remarks and IP1: Semi-parametric Inference: A Bayesian Curse?

In this talk I will discuss some issues around Bayesian approaches in semiparametric inference. I will first recall some positive and negative results on Bernstein von Mises theorems in non-and semi-parametric models. I will then propose two possible tricks to derive posterior - type distributions in semiparametric models which allow both for efficient procedures and Bernstein von Mises theorems, as well as flexible priors on the nonparametric part. The first approach, based on the cut posterior will be illustrated in semi-parametric mixture and Hidden Markov models and second, a targeted posterior, will be applied in the well-known causal inference problem of average treatment effect estimation. This talk is built on joint works with Edwin Fong, Chris Holmes, Dan Moss and Andrew Yiu.

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IP2

Exploiting Low-Dimensional Structure in Bayesian Inverse Problems Governed by Ice Sheet Flow Models

Model-based projections of complex systems will play a central role in prediction and decision-making, e.g., anticipate ice sheet contribution to sea level rise. However, models are typically subject to uncertainties stemming from uncertain inputs in the model such as coefficient fields, source terms, etc. Refining our understanding of such models requires solving a (Bayesian) inverse problem that integrates measurement data and the model to estimate and quantify the uncertainties in the parameters. Such problems face several challenges, e.g., high dimensionality of the inversion parameters and expensive to evaluate models. In this talk, I will focus on identifying and exploiting low-dimensional structure in such inverse problems stemming for example from local sensitivity of the data with respect to parameters, diffusive models, sparse data, etc. The key idea is to look at the Hessian operator arising in these inverse problems, which often exhibits a low rank and even a lower off-diagonal structure, and build approximations of this operator which can be used as preconditioners for the Newton-Krylov systems or to build more-informative proposals in an MCMC context. Combining an efficient matrix-free point spread function (PSF) method for approximating operators with fast hierarchical (H-)matrix methods, we show that Hessian information can be obtained using only a small number of operator applications.

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IP3

Wasserstein Distributional Learning

Learning function-on-scalar predictive models for conditional densities and identifying factors that influence the entire probability distribution are vital tasks in many data-driven applications. Conventional approaches work mostly with summary statistics and are hence inadequate for a comprehensive investigation. We present an efficient Majorization-Minimization optimization algorithm, Wasserstein Distributional Learning (WDL), that trains Semi-parametric Conditional Gaussian Mixture Models (SCGMM) for conditional density functions and uses the Wasserstein distance as a proper metric for the space of density outcomes. We further provide theoretical convergence guarantees and illustrate the algorithm using boosted machines. Experiments on the synthetic data and real-world applications demonstrate the effectiveness of the proposed WDL algorithm.

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IP4

Computational Hypergraph Discovery, a Gaussian Process Framework for Connecting the Dots

Most scientific challenges can be framed into one of the following three levels of complexity of function approximation.

- Type 1: Approximate an unknown function given input/output data.
- Type 2: Consider a collection of variables and functions, some of which are unknown, indexed by the nodes and hyperedges of a hypergraph (a generalized graph where edges can connect more than two vertices). Given partial observations of the variables of the hypergraph (satisfying the functional dependencies imposed by its structure), approximate all the unobserved variables and unknown functions.
- Type 3: Expanding on Type 2, if the hypergraph structure itself is unknown, use partial observations of the variables of the hypergraph to discover its structure and approximate its unknown functions. Although Gaussian Process (GP) methods are sometimes perceived as a well-founded but old technology limited to Type 1 curve fitting, they can be generalized to an interpretable framework for solving Type 2 and Type 3 problems, all while maintaining the simple and transparent theoretical and computational guarantees of kernel/optimal recovery methods.

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IP5

Statistical Divergences for Functional Data

Kernel-based discrepancies have found considerable success in constructing statistical tests which are now widely used in statistical machine learning. Examples include Kernel Stein Discrepancy which enables goodness-of-fit tests of data samples against an (unnormalized) probability density based on Stein's method. The effectiveness of the associated tests will crucially depend on the dimension of the data. I will present some recent results on the behaviour of such tests in high dimensions, exploring properties of the statistical divergence under different scaling of data dimension and data size. Building on this, I will discuss how such discrepancies can be extended to probability distributions on infinite-dimensional spaces. I will discuss applications to goodness-of-fit testing for measures on function spaces and its relevance to various problems in UQ.

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IP6

Optimal State and Parameter Estimation Algorithms

In this talk, I will present an overview of recent works aiming at solving inverse problems (state and parameter estimation) by combining optimally measurement observations and parametrized PDE models. After defining a notion of optimal performance in terms of the smallest possible reconstruction error that any reconstruction algorithm can achieve, I will present practical numerical algorithms based on nonlinear reduced models for which we can prove that they can deliver a performance close to optimal. The proposed concepts may be viewed as exploring alternatives to Bayesian inversion in favor of more deterministic notions of accuracy quantification.

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IP7

Closing Remarks and IP7: A Surrogate Modeling Journey through Gaussian Processes Modeling for Computer Simulation Experiments

This talk begins with an overview of Gaussian process (GP) surrogate modeling, and my favorite application: active learning for the (Bayesian) optimization of a black-box function. I shall then survey some important, recent methodological developments targeting specific situations that increasingly arise in practice: large simulation campaigns, noisy observations/stochastic simulation, nonstationary modeling, and the calibration of computer models to field data. The presentation concludes with an in-depth description of a recent application: contour location for reliability in an airfoil simulation experiment using deep GPs. Throughout, there will be reproducible visuals and demos supported by code, both run live and embedded in the slides. These are biased toward my own work, in part because I understand that code best. But along the way I shall also endeavour to provide an otherwise balanced discussion of myriad alternatives that can be found elsewhere in this fast-moving literature.

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SP1

SIAG/Uncertainty Quantification Early Career Prize Lecture - Perspectives on Stochastic Gradient Descent

The stochastic gradient descent (SGD) algorithm has been a staple in stochastic optimisation, the control of stochastic systems, and probably most prominently the training of deep neural networks. SGD allows to replace expectations in target functions by sample averages and, hence, sums over large data sets by sums over small subsampled data sets. Thus, stochastic optimisation problems become computationally accessible, machine learning problems become scalable. In deep learning, SGD has further objectives: the stochasticity aims to 'implicitly regularise the problem, it allows the trajectory to overcome local minimisers in nonconvex target functions, and it possibly even quantifies uncertainties. In this talk, we discuss stochastic gradient descent in machine learning and analyse it using a novel continuous-time formulation. Here, we have a particular focus on implicit regularisation and uncertainty quantification.

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CP1

Calibration with Unknown Discrepancy

In order to calibrate the input parameters of an expensive simulator (whether via Bayesian calibration or history matching), its important to account for model discrepancy, and ignoring or mis-specifying this can affect inference about the inputs x. However setting this discrepancy may be difficult, particularly if the model output is high-dimensional, and it may be challenging to directly elicit its form from an expert. To remove this prior requirement, we reframe the calibration problem as searching for informative (about reality) simulations. Instead of using a discrepancy-dependent distance metric, we combine an emulator of the expensive simulator with a model representing the experts judgement about particular model simulations, rather than over the discrepancy directly. As with the history matching framework, we iteratively remove parts of the input parameter space that are inconsistent with or uninformative about reality. Over several iterations, we explore and refine not ruled out space, guided by expert judgement over what informative simulations look like, and identifying regions of the input space that lead to model output consistent with this judgement.

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CP1

Sequential Experimental Design for Materials Strength Model Calibration

Due to the time and expense associated with physical experiments, there is significant interest in optimal selection of the conditions for future experiments. Selection based on reduction in parameter uncertainty provides a natural path forward. We consider this type of optimal sequential design in the context of Bayesian calibration of materials strength models with the strength model characterizing the evolving resistance of a material to permanent strain. This problem is particularly challenging because different types of experiments and associated diagnostics are employed across strain rate regimes. For lower-strain-rate experiments, stress-strain curves can be measured directly. For higher-strain-rate experiments, strength must be inferred (e.g., from the deformation of a cylinder of material in a Taylor cylinder experiment). We employ data fusion in our sequential design methodology to incorporate these multiple experimental modalities. LLNL-ABS-835231 This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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CP1

Solving High-Dimensional, PDE-Based, Bayesian Inverse Problems by Beyond-Black-Box Saddle Point Optimization

We propose a novel Bayesian formulation for high-dimensional, PDE-based, inverse problems. Traditional methods scale poorly in terms of the number of expensive likelihood evaluations, i.e. black-box forward-model calls, needed when the number of unknowns increases. We tackle this problem while still keeping the advantages of Bayesian formulations, i.e. the ability to handle stochastic noise and provide probabilistic estimates. To this end, we bypass the evaluations of the forward model by breaking open the black-box. Thus, we use the governing equations (PDEs) in the form of weighted residuals and incorporate them in a virtual likelihood term. We formulate a saddle point problem, where we only consider the single, most significant weighted residual as a virtual observable. The method involves iterating between a) finding the weight function that yields the largest mean square residual, and b) optimizing the parameters of our approximate posterior using stochastic variational inference. Instead of expensive forward-model calls, we compute a single integral over the problem domain at each iteration, thus enabling a rapid approximation of the posterior. Finally, we demonstrate that our formulation does not even require setting up a well-posed forward problem in order to solve the inverse problem and illustrate its capabilities in applications from linear elasticity and diffusion problems.

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CP2

Virtual Data-Driven Probabilistic Surrogates for Parametrized PDEs

The cost of repeatedly solving a PDE under different parametric inputs is the main computational bottleneck in many-query applications such as uncertainty quantification and model-based optimization. Data-driven strategies have risen in prominence in recent years and several techniques have been proposed which circumvent the need of generating an expensive training dataset of input-output pairs by employing residuals of the PDE in the loss function. We propose a fully probabilistic approach in which the governing PDE is treated as a source of virtual data which is probed using weighted residuals. We formulate this as a stochastic Variational Inference objective, the output of which is a mesh-free, probabilistic surrogate. Learning is enhanced by introducing information bottlenecks in order to overcome the potentially very high-dimension of the parametric inputs as well as of the PDE solution we wish to predict. We demonstrate the efficacy of the proposed scheme under various settings for elliptic, parametric PDE and compare with state-of-the-art alternatives.

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CP2

Multifidelity Approaches for Solving Inverse Problems Relying on Computer Codes with Functional Outputs - Application to Thermal Evaluation of Buildings

The thermal insulation of buildings, indicated by the thermal resistance of their walls, is a key factor in ensuring the thermal comfort of occupants and achieving significant energy savings. The work to be presented focuses on identifying the thermal resistance of highly insulated walls. To accomplish this, a Bayesian sequential multi-fidelity statistical approach will be developed to automatically select the most appropriate version of either the physical model or surrogate model at each iteration of the inversion algorithm. This model represents the best compromise between computational cost and the expected reduction in uncertainty, accurately identifying the thermal resistance of a given wall. To achieve this goal, an original problem formulation will be used to minimize the influence of uncontrolled variables (such as heat exchange coefficients between the wall and the exterior, the initial state of the wall, etc.), and a Bayesian formulation will be applied to incorporate model and measurement uncertainties in the thermal resistance estimation process. This protocol is tested on a 4-layer wall with highly interior insulation, utilizing temperature and flux simulations based on 0D, 1D, and 2D physical wall models.

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CP2

Modeling Joint Wind Speed Distributions in Wind Farms Using Copulas

Abstract Wind farm analysis is crucial for optimizing renewable energy generation and operational efficiency. One challenge is accurately modeling the joint distribution of wind speeds across different wind farms to capture their interdependence. This paper proposes a copula-based approach to constructing multivariate distributions for pairs of wind farms. The method begins by fitting Weibull distributions to individual wind farm data and subsequently builds a covariance matrix based on the training dataset. A Gaussian copula is then employed to model the dependency structure between the wind farms. By incorporating correlations into the marginal distributions, the approach can generate joint distributions that better capture real-world wind speed behaviors. The proposed methodology is presented alongside code implementations for clarity. The paper discusses the potential challenges associated with the Gaussian copula and introduces avenues for exploring

alternative copulas to account for more complex dependency patterns. The performance evaluation of the resulting multivariate distribution is also examined using metrics like cross entropy and KL divergence. The proposed approach offers a systematic framework for addressing wind farm analysis challenges by providing a flexible and efficient means of modeling multivariate wind speed distributions, facilitating improved decision-making and operational strategies in renewable energy applications.

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CP3

Integrating the Lagrange Energy Method with the Degradation Constitutive Modelling for Biomaterial Analysis

The Deep Ritz method was introduced for solving high-dimensional partial differential equations [E. Weinan, The deep Ritz method: A deep learning-based numerical algorithm for solving variational problems], was extended to the field of mechanical calculations for hyperelastic materials, leading to the development of the Deep Energy Method [Vien Minh Nguyen-Thanh, A deep energy method for finite deformation hyperelasticity]. A Lagrange Energy method is proposed to combine the benefits of the finite element method in applying the Dirichlet boundary conditions. The elastic energy across the entire domain is computed and integrated to serve as the system's energy loss function for optimising the global displacement. Our work has integrated the Lagrange Energy Method with a biomaterial constitutive model considering degradation effects [Malte Rolf-Pissarczyk, A discrete approach for modelling degraded elastic fibres in aortic dissection]. A stochastic Gaussian process is employed to generate a random field of degradation coefficients [Sascha Ranftl, Stochastic modelling of inhomogeneities in the aortic wall and uncertainty quantification using a Bayesian encoder-decoder surrogate]. These coefficients are incorporated into the forward calculation process for the energy density field. Following energy integration and backward optimisation, the displacement and the stress field are evaluated.

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CP3

An Adaptive Regularized Rom for the Quasi-Geostrophic Equations

We propose a novel regularized Reduced Order Model (ROM) for the Quasi-Geotrophic Equation. Regularization techniques are often used to improve the reconstructed solution accuracy when the Kolmogorov n-width is typically high and the number of modes to be considered to capture all the main features of the dynamical system is much high. In "[Girfoglio et al., A linear filter regularization for pod-based reduced-order models of the quasi-geostrophic equations, Comptes Rendus. Mecanique, 2023]" the authors proposed a linear filtering-based Large Eddy Simulation (LES) approach. In this work, we intend to improve what is done in "[Girfoglio et al., A linear filter regularization for pod-based reduced-order models of the quasi-geostrophic equations, Comptes Rendus. Mecanique, 2023]" by employing a nonlinear low-pass filter. We propose and compare several nonlinear data-driven approaches to learn the filtering radius associated with the LES model. The potential of the proposed data-driven techniques is demonstrated on the classical double-gyre wind forcing benchmark case. We will show that our regularized ROM is able to retain the solution accuracy even when a few eigenmodes are considered as compared to the standard ROM, i.e., without any regularization.

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CP4

Nth Moments of Multivariate Hermite Polynomials in Correlated Gaussian Parameters

In uncertainty quantification, polynomial chaos methods are sampling-free techniques used to approximate the solution of a stochastic partial differential equation (PDE). The solution is represented by a polynomial expansion truncated to finitely many terms, whose deterministic coefficient functions are recovered through Galerkin projections. In the presence of multiple uncertainties, the projection step introduces products (Nth moments) of the basis functionals, where N is the degree of nonlinearity of the governing PDE. When these uncertainties are given by correlated random variables, there is no closed-form expression for these products, even when the uncertainties have a joint Gaussian distribution. Consequently, the products the number of which grows exponentially due to the curse of dimensionality are typically computed via repeatedly drawing realizations from the Gaussian distribution, which can (a) become computationally expensive to implement, and (b) introduce errors if the sample count is insufficient. In previous work, a new expression was found for the simple and efficient evaluation of the double products (second order moments) of the basis polynomials (multivariate Hermite) with correlated Gaussian inputs. We present an iterative formula for the Nth order products in terms of lower-order moments. This formula will allow polynomial chaos methods to be more readily applied to solving stochastic nonlinear PDEs with correlated Gaussian parameters.

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CP4

Spatially Correlated Sampling From Parallel Partial Emulators

Parallel partial emulators (PPEs) offer quick and accurate approximations of complex computer models with high-dimensional spatial outputs. In a recent preprint, Gao and Pitman show that PPE mean predictions inherit conservation properties from model simulations. Yet as PPEs assume independence amongst output dimensions, spatially correlated samples are not available. To overcome this issue, we use linked Gaussian process emulators to approximate PPE covariance over both input dimensions and space. We apply this method to two common advection-diffusion models: Burgers and Richards equations.

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CP5

Conformal Prediction for Surrogate Modelling with Gaussian Processes

Conformal Prediction (CP) has gained prominence as a method for a sort of uncertainty quantification of machine learning models [Vovk et. Al, Algorithmic learning in a random World, 2005]. Assuming basic data exchangeability (e.g., i.i.d), CP allows to construct prediction sets with formal probabilistic coverage guarantees. For scalar outputs, CP provides prediction intervals for any confidence level $\alpha \in (0, 1)$, going beyond point predictions. This talk will introduce CP principles and cross-conformal estimators [Barber et. Al, Predictive inference with the jackknife+, 2021]. We then investigate the performance of surrogate models of simulation codes by combining CP cross-conformal estimators with Gaussian Process regressors [Rasmussen et. Al, Gaussian Processes for Machine Learning, 2006]. This yields adaptive prediction intervals that are correlated to the model error without assuming additional hypothesis. Numerical experiments on both simple and industrial models will be shown where more robust conceptual and quantitative results for uncertainty quantification of GP metamodels are achieved.

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CP5

Sparse Grid Stochastic Collocation Methods and Spatial Adaptivity

We present an adaptive algorithm for the computation of quantities of interest of random elliptic partial differential equations. We consider a PDE problem where the source of randomness is given by a diffusion coefficient that is parametrized by means of a Kahunen-Love expansion. One common approach is to restrict the countably infinite dimensional parameter space to a finite-dimensional parameter set and subsequently apply a spatial discretization and an approximation in the parametric variables. In our method, we use a dimension-adaptive sparse grid approach to balance a stochastic collocation method with a finite element approximation. For this spatial discretization, we apply an adaptive finite elements method which allows us to adjust to the spatial regularity of the problem. Our adaptive algorithm uses the benefit-cost ratio to steer the adaptive process in the dimension-adaptive combination technique and to balance cost and error of the discretization steps. In order to define a hierarchy of spatial discretizations, we consider error tolerances and construct non-uniform meshes using suitable adaptive finite element error estimators. We include numerical examples which show good performance of the algorithm, even when spatial singularities are present.

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CP5

Hierarchical Matrix-Based System Reliability Method for Large-Scale Systems

Reliability analyses of large-scale systems under natural or human-made hazards often face formidable challenges, including immense computational costs. The matrix-based system reliability (MSR) method (Song and Kang, 2009) facilitates the failure probability calculations of general system events by its matrix-based formulation based on basic mutually exclusive and collectively exhaustive events. However, the practical application of the MSR method can be limited for systems with many components or significant statistical dependencies between component failure events. In this study, a hierarchical MSR (hMSR) is proposed to mitigate the limitations by employing a divide-and-conquer approach. The hMSR method consists of a probability-updating algorithm to capture statistical dependencies and a data-storage method tailored for the hierarchical structure. The proposed method enables efficient reliability analysis of large-scale systems, which was restricted in the original MSR method because of memory demands, and probabilistic inference for given observations of specific components or subsystem states. The performance of the hMSR method is tested and demonstrated virtual system examples in comparison to the original method. Furthermore, various conditional probability-based importance measures are computed for components in large-scale gas plant systems using the hMSR method.

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CP5

Augmented Quantization: a General Approach to Mixture Models

The investigation of mixture models is a key to understand and visualize the distribution of multivariate data. Most mixture models approaches are based on likelihoods, and are not adapted to distribution with finite support or without a well-defined density function. This study proposes the Augmented Quantization method, which is a reformulation of the classical quantization problem but which uses the p-Wasserstein distance. This metric can be computed in very general distribution spaces, in particular with varying supports. The clustering interpretation of quantization is revisited in a more general framework. The performance of Augmented Quantization is first demonstrated through analytical toy problems. Subsequently, it is applied to a practical case study involving river flooding, wherein mixtures of Dirac and Uniform distributions are built in the input space, enabling the identification of the most influential variables.

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CP6

MUSE, a Stochastic Tool for Modeling Spatial Uncertainty as Support for Multi-scenario Application in Environments

Modeling the complexity of natural environments can be addressed through numerical approximations. In this context, uncertainty quantification becomes fundamental to assess the degree of reliability of the final model. Our research intends to implement theory into practice through a methodology with a general approach. It is conceived to work in various application fields, where the estimation of the spatial distribution of one or more variables should be tailored over the size of the survey area and over the geometrical features. Exploiting features of regionalized variables, after the evaluation of models of spatial dependence by variograms computation, the spatial uncertainty is quantified to be used in a decision support system. The code implementing geostatistical theory is a stochastic open-source tool aiming to be ready in Modeling Uncertainty as Support for multi-scenario application in Environments or briefly MUSE. Interesting results are obtained by using MUSE computational code on different case studies, highlighting its potential for calculation and flexibility in different scenarios, varying from modeling complex geologies, to applications in geochemistry.

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CP6

Bayesian Directed Sampling for Efficient Conditional Validation of Low-Order Models and Model Sets

Typical approaches to supervised classification make two broad assumptions: that large quantities of data are available, and that the data are categorical. In contrast, in many engineering applications collecting data is slow and expensive, but test results are information-rich. To bridge this gap, we propose an algorithm that uses real-valued labels to estimate a system's valid set—that is, the set of conditions over which the labels are positive. By using a Gaussian process to model gradients and uncertainties, our algorithm directs function sampling to greedily minimize the expected posterior misclassification rate at each step. In testing against 500 random functions drawn from a $\sigma = 1$ two-dimensional Gaussian process prior, our algorithm's directed sampling reaches an average misclassification rate of 0.026% in only 50 samples, while a support vector machine trained on undirected sampling (either a uniform grid or a uniform random sample) reaches an average misclassification rate of 4.4% with the same sample size. This method has applications in conditional validation of low-order models of complex systems, and can be extended to validate sets of models, with sample complexity increasing sublinearly with the number of models.

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CP6

To Spike Or Not to Spike: the Whims of the Wonham Filter in the Strong Noise Regime

We study the celebrated Shiryaev-Wonham filter in its historical setup of Wonham (1964) where the hidden Markov jump process has two states. We are interested in the weak noise regime for the observation equation. Interestingly, this becomes a strong noise regime for the filtering equations. Earlier results of the authors show the appearance of spikes in the filtered process, akin to a metastability phenomenon. This paper is aimed at understanding the smoothed optimal filter, which is relevant for any system with feedback. In particular, we demonstrate that there is a sharp phase transition between a spiking regime and a regime with perfect smoothing.

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CP6

End-To-End Uncertainty Quantification with Analytical Derivatives for Design Under Uncertainty

Uncertainty quantification (UQ) is a rapidly growing and evolving discipline, especially within the aerospace community. Performing analysis with UQ can provide decision makers with a wealth of information about a candidate de-

sign. However, the value of UQ is fully realized when the information gained during UQ analysis is leveraged in a feedback loop of a design optimization process, often referred to as design under uncertainty. Although design under uncertainty can be a powerful risk mitigation technique, there are a number of roadblocks that prevent its implementation. Two primary factors are computational costs and added complexity of the analysis. High fidelity simulations on the order tens of uncertain variables quickly become computational infeasible. Also, implementing UQ into an existing multidisciplinary design and optimization (MDO) process often requires extensive knowledge of the UQ methods and careful treatment of the problem formulation. The objective of this work is to address these two primary roadblocks and enable practitioners to efficiently perform design under uncertainty with limited knowledge of the UQ discipline. Methods outlined in this paper demonstrate MDO incorporating UQ into the design process, leveraging an analytic derivative tool chain through the entire optimization. The proposed approach leverages novel machine learning techniques to generate a differentiable confidence interval output from polynomial chaos models.

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CP7

Uncertainty Quantification and Sensitivity Analysis of Co-Kurtosis PCA for Dimensionality Reduction in Combustion Modeling

For multi-scale multi-physics applications e.g., the turbulent combustion code Pele, robust and accurate dimensionality reduction is crucial to solving problems at exascale and beyond. A recently developed technique, Co-Kurtosis based Principal Component Analysis (CoK-PCA) which leverages principal vectors of co-kurtosis, is a promising alternative to traditional PCA for complex chemical systems. To improve the effectiveness of this approach, we employ Artificial Neural Networks for reconstructing thermochemical scalars, species production rates, and overall heat release rates corresponding to the full state space. Our focus is on bolstering confidence in this deep learning based non-linear reconstruction through Uncertainty Quantification (UQ) and Sensitivity Analysis (SA). UQ involves quantifying uncertainties in inputs and outputs, while SA identifies influential inputs. One of the noteworthy challenges is the computational expense inherent in both endeavors. To address this, we employ the Monte Carlo methods to effectively quantify and propagate uncertainties in our reduced spaces while managing computational demands. Our research carries profound implications not only for the realm of combustion modeling but also for a broader audience in UQ. By showcasing the reliability and robustness of CoK-PCA in dimensionality reduction and deep learning predictions, we empower researchers and decision-makers to navigate complex combustion systems with greater confidence.

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CP7

Improved High-Dimensional Covariance Matrix Estimation in Cross-Entropy Scheme for Rare Event Analysis

A popular adaptive importance sampling scheme in rare event analysis is the Cross-Entropy (CE) scheme. It is known to succumb to the weight degeneracy phenomenon in high-dimensional setting. In Gaussian setting where the auxiliary density is parameterized by its mean and covariance matrix, the optimal covariance matrix possesses a smallest eigenvalue that takes low values. CE attempts to estimate iteratively the optimal covariance matrix through empirical covariance matrix estimators. However, with a reasonable number of samples per iteration, the empirical estimators often underestimate the smallest eigenvalue of the optimal covariance matrix, cascading into weight degeneracy within the next few iterations of CE. We propose to adapt the Nonparametric Eigenvalue-Regularized COvariance Matrix Estimator (NERCOME) into CE. NERCOME increases the smallest eigenvalue by decoupling the estimated eigenvalues and eigenvectors from the empirical estimators, therefore suitable for application into CE in order to avoid weight degeneracy. To further mitigate against the high dimensionality, NERCOME is projected onto its reduced eigenspace formed only by a select few eigenvectors, with their eigenvalues ranked increasingly according to $x \mapsto \log(x) - x + 1$, as suggested by recent results. Some improvements on the probability estimation of several test cases up to dimension 300 have been obtained.

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CP7

A Sampling Method for Minimizing the Expectation of Multiple Random Objectives

Solving optimization problems with multiple objectives consisting of expectations of random quantities can be challenging. The difficulty arises from a) the evaluation of the averaged objectives and b) their comparison to determine the Pareto front (set of optimal solutions). Stochastic gradient approaches alleviate the need for costly expectation computations during minimization while converging to non-dominated designs. However, we show that standard stochastic gradient approaches introduce a bias, causing convergence toward a subset of optimal designs and not the whole of the Pareto front. We propose an improved stochastic gradient approach that incorporates a bias reduction and a noise term designed to ensure the exploration of the whole Pareto front. Specifically, we rely on a local averaging procedure, calibrated using spatial autocorrelation, and a Markov-Chain with a diffusion term restricted to the direction tangential to the front. Since this stochastic gradient method generates samples in the neighborhood of the Pareto front we also propose an analysis of the samples to estimate the Pareto front with valid

confidence intervals. This estimation is based on local averaging and ranked fitness of the samples. We demonstrate the proposed approach numerically on simple problems and discuss its extension to engineering applications.

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CP8

Deep Neural Networks Coupled Finite Element for Evolution Equations

In this work we present a novel approach that combines deep neural networks with the finite element method for solving evolution partial differential equations (PDEs). In contrast to the conventional approach of directly approximating the solution within a spatiotemporal domain using neural networks, our methodology involves representing the solution as a tensor product. Specifically, we express it as a composition of a sequence of fixed local finite element basis functions in the temporal domain and an array of unknown neural networks in the spatial domain. The efficiency of our proposed method is empirically demonstrated through a series of numerical experiments.

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CP8

Multilevel Markov Chain Monte Carlo with Likelihood Scaling for Full-Field Data Assimilation in Structural Health Monitoring

In recent years, the development of new observation techniques in various branches of engineering disciplines has created the possibility of generating full-field data on systems under study. An example of this is Digital Image Correlation in structural mechanics, which allows for full-field vibration measurements of civil engineering structures. In some cases, however, the resolution of this full-field data is so high that the computational cost of using this data to solve Bayesian inverse problems becomes prohibitively expensive. While the incorporation of expensive forward models in a data assimilation context has recently been addressed by the multilevel Monte Carlo methodology, the standard setting still assumes that measurement data is only available in selected measurement points. In this talk, we show a successful generalisation of a multilevel Markov Chain Monte Carlo algorithm within the context of structural health monitoring using full-field vibration data. The method reduces computational efforts by allowing the resolution of the data to vary across levels, along with the resolution of the forward model. We discuss our results and show that the data can be scaled in a simple way to decrease the cost of likelihood evaluation at the coarser levels.

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CP9

Data-Driven Digital Twin of Dynamical Systems by a Probabilistic Narmax Model

The digital twin (DT) of a dynamical system is essential to predict the systems behaviour in real-time or future times. A nonlinear autoregressive moving average with exogenous input (NARMAX) model has been used in our study to formulate DT of dynamical systems. To take into account the noisy behaviour of the collected data (i.e., responses), the NARMAX model parameters were modelled using Bayesian inference. The Bayesian model parameters were represented in a Forney-style factor graph, and it was used for updating posterior distributions for a set of parameters governing the output response. A variational Bayesian message-passing algorithm was used to infer the posterior distribution for the Bayesian model parameters. The developed framework has been used to formulate DT for a single degree of freedom and a multi-degree of freedom dynamical systems. For both systems, the DT was formulated based on limited input and output data. Furthermore, future responses were predicted by the probabilistic NARMAX model for a long time, and the predicted results were found to be quite accurate to the actual simulated responses. In addition, the probabilistic regime was also predicted, which has been calculated from the posterior distribution of the Bayesian model parameters. The probabilistic regime was useful in predicting the behaviour of the noise in the system.

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CP9

A Study of Distributionally Robust Mixed-Integer Programming with Wasserstein Metric: on the Value of Incomplete Data

This study addresses a class of linear mixed-integer programming (MILP) problems that involve uncertainty in the objective function parameters. The parameters are assumed to form a random vector, whose probability distribution can only be observed through a finite training data set. Unlike most of the related studies in the literature, we also consider uncertainty in the underlying data set. The data uncertainty is described by a set of linear constraints for each random sample, and the uncertainty in the distribution (for a fixed realization of data) is defined using a type-1 Wasserstein ball centered at the empirical distribution of the data. The overall problem is formulated as a three-level distributionally robust optimization (DRO) problem. First, we prove that the three-level problem admits a single-level MILP reformulation, if the class of loss functions is restricted to biaffine functions. Secondly, it turns out that for several particular forms of data uncertainty, the outlined problem can be solved reasonably fast by leveraging the nominal MILP problem. Finally, we conduct a computational study, where the out-of-sample performance of our model and computational complexity of the proposed MILP reformulation are explored numeri-

cally for several application domains.

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CP10

Sensitivity-Based Uncertainty Quantification for Plasma Edge Codes for Nuclear Fusion Reactors

Plasma edge codes are currently the main tools for interpreting the plasma boundary behavior in fusion experiments, and for designing future reactors. These codes are complex and computationally expensive, coupling a multifluid model for the plasma with a kinetic model for the neutral particles. Moreover, several uncertainties are present throughout the complex simulation chain. Therefore, uncertainty quantification (UQ) for model validation with plasma edge codes appears a challenging task, which is presently precluded by the high computational costs. In this contribution, we show how adjoint sensitivity analysis enables UQ for plasma edge codes, discussing achievements and remaining challenges. To obtain adjoint sensitivities in a complex and continuously developed code we employ Algorithmic Differentiation. Such sensitivities are then fed to gradient-based optimization methods, which are employed to solve the backward UQ problem. Casting the backward UQ into a Bayesian MAP setting, we consistently account for information and uncertainties from different diagnostics. Finally, we show how the in-parts adjoint technique allows sensitivity propagation throughout the whole simulation chain, including the magnetic field upon which the plasma grid is based.

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CP10

Gaussian Process Regression for High Dimensional Graph Inputs

In many science and engineering fields, mesh-based numerical methods are traditionally leveraged for solving partial differential equations that describe some physical systems. While mesh-based approaches provide high-fidelity approximations, they remain prohibitively expensive and difficult to exploit in real-life industrial processes. In this work, we are concerned with learning mesh-based simulations in the presence of both geometric and parametric variabilities in the underlying physical system of interest. We rely on Gaussian process meta-models on high-dimensional graph spaces for optimization and uncertainty propagation purpose. To this end, we introduce the Sliced Wasserstein Weisfeiler-Lehman (SWWL) graph kernel function. In contrast to many existing graph kernel functions, the proposed SWWL kernel enjoys positive definitess and a drastic complexity reduction. The new kernel is first validated on graph classification tasks which involve molecular datasets made of small graphs. The efficiency of the SWWL kernel is then illustrated on graph regression tasks in the fields of computational fluid dynamics and solid mechanics, where the input graphs are made of several thousand nodes.

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CP11

Efficient Importance Sampling of Piecewise Deterministic Markov Processes with a Graph-Based Adaptive Procedure

Our objective is to estimate the probability that a trajectory of a Piecewise Deterministic Markov Process (PDMP) reaches a target region in its state space before a fixed time. We focus on the rare event framework where the target region is rarely visited, resulting in a small target probability. A typical application is when the PDMP models a complex dynamic industrial system, and the target region corresponds to system failure. An estimator with zero variance of the target probability can be produced by an importance sampling method, provided we have knowledge of the 'committor function' of the process. The committor function represents the probability of reaching the target region given the current state of the trajectory. We propose a method for the sequential approximation of this committor function. First, we explicitly compute the mean hitting times of a random walk on a graph that mimics the PDMP. We deduce from these times a family of approximations of the committor function resulting in a parametric family of importance distributions. The parameter of this family is then sequentially optimized through a cross-entropy procedure. These successive importance distributions produce increasingly accurate estimators of the target probability. The method is applied to a system from the nuclear industry.

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CP11

Estimation of Large Covariance Matrices via Free Deconvolution: Computational and Statistical Aspects

The estimation of large covariance matrices has a high dimensional bias. Correcting for this bias can be reformulated via the tool of Free Probability Theory as a free deconvolution. The goal of this work is a computational and statistical resolution of this problem. Our approach is based on complex-analytic methods methods to invert S-transforms. In particular, one needs a theoretical understanding of the Riemann surfaces where multivalued S-transforms live and an efficient computational scheme.

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CP11

Uncertainty Quantification for Band-Limited Functions

Functions whose Fourier transforms have compact supports, called band-limited, are widely used in various engineering fields, especially in signal processing. According the well-known Nyquist-Shannon sampling theorem, if we have a deterministic (discrete) equidistant sample from this function having a sampling rate at least twice the bandwidth (Nyquist rate), then the function can be perfectly reconstructed from the sample. It this talk we investigate the cases, when we only have a finite dataset randomly sampled from a (potentially unknown) input distribution, and the outputs of the target (band-limited) function can also have measurement noises. We suggest algorithms for these four cases, i.e., known / unknown input distribution, and function values with / without measurement noises, which are able to construct simultaneous confidence bands for the underlying true (regression) function under very mild statistical assumptions; they are essentially distribution-free. We present non-asymptotic theoretical guarantees for the cases of known input distributions (unknown measurement noises can still affect the outputs). For the case of unknown input distributions, the confidence bands are asymptotically guaranteed. We argue that all of these (four) methods are uniformly strongly consistent, i.e., they shrink around the true function and in the limit they cannot contain any other functions, almost surely. Finally, we illustrate the approaches via a series of numerical experiments.

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CP12

Variational Autoencoder with Weighted Samples for High-Dimensional Non-Parametric Adaptive Importance Sampling

Probability density function estimation with weighted samples is a major topic of interest in statistics. In particular, it is the main foundation of all adaptive importance sampling (IS) algorithms. Classically, a target distribution is approximated either by a non-parametric model or within a parametric family. However, these models suffer from the curse of dimensionality or from their lack of flexibility. In this contribution, we suggest to use as the approximating model a distribution parameterised by a variational autoencoder (VAE). We extend the existing framework of VAEs to the case of weighted samples by introducing a new objective function. The flexibility of this family makes it close to a non-parametric model, and despite the very high number of parameters to estimate, this family is much more efficient in high dimension than the classical Gaussian or Gaussian mixture families. Moreover, in order to add flexibility to the model and to be able to learn multimodal distributions, we use a learnable prior distribution for the latent variable. We also introduce a new pre-training procedure for the VAE to find good starting weights of the neural networks to prevent as much as possible the posterior collapse phenomenon to happen. At last, we explicit how to use the resulting distribution in an IS context, and we introduce the proposed procedure in an adaptive IS algorithm to estimate a rare event probability in high dimension on two multimodal problems.

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CP12

Uncertain Domains and Computations for PDE Problems Based on Fictitious Domain FEMs

We investigate PDE problems defined on uncertain domains and discretized by a fictitious domain finite element method. Key ingredients of the study are to manage cases considering the usually computationally forbidden combination of poorly conditioned equation system matrices due to challenging geometries, possible optimal control searches with iterative methods, slow convergence to system solutions on deterministic and non-deterministic levels, and expensive remeshing due to geometrical changes. We overcome all these difficulties, utilizing the advantages

of proper preconditioners adapted to unfitted mesh methods, improved types of Monte Carlo methods, and mainly employing the embedded FEMs advantages combined with new efficient model order reduction techniques, based on a fixed background mesh computed once even if geometrical changes are taking place.

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CP13

Robust and Mixture Gp Surrogates in Small Data Regimes

For many UQ tasks it is first necessary to build a surrogate from a set of expensive calls to a detailed computer code. Gaussian Processes (GP) are ubiquitous for surrogate modeling, as they are flexible emulators and naturally embed a measure of the precision that can be expected from their predictions. This measure can be a means of 'quantifying the robustness' of the surrogate. Yet, such feature has to be considered carefully in small data regimes resulting from computer budget constraints or a large dimension of the design space. For tractability, both the identification and exploitation of the GP model often rely on a single best value of the GP parameters, usually obtained through likelihood maximization. With few data, different parameter values may constitute credible options, from a bayesian perspective. This may lead to unstable results and to over-confidence in the GP prediction capabilities. Here, it is proposed to compare several GP building strategies for UQ purposes, in small data regimes. Specifically we consider Gaussian mixture predictors obtained from a Bayesian Model Average (BMA) over of a pool of different GP candidates. This embodies a compromise between a potentially unstable single GP estimate and a more robust yet poorly tractable 'fully-bayesian GP', where a prediction is obtained from marginalization over the posterior on GP parameters, the latter being computed from the available data set and a user-defined prior.

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CP13

Nested Importance Sampling for Bayesian Inference with Expensive, Black-Box Likelihood Functions

Monte Carlo sampling methods are fundamental to the application of Bayesian system identification, but can be infeasible for computationally expensive black-box likelihood functions and may be unable to deal with complex, multimodal posteriors, that are often encountered in engineering applications. We propose an approach for performing nested importance sampling, combined with a Gaussian process based surrogate model of the likelihood function. Building on the recent work of [M. J. Williams et al. (2023) - Importance nested sampling with normalising flows], our approach aims to simultaneously optimize a sequence of proposal distributions that generate weighted samples from the posterior with progressively higher likelihoods, and utilizes kernel density estimation to approximate the intractable evidence integral. An active learning scheme is employed to iteratively select the optimal points where the likelihood function will be evaluated. The proposed approach displays an increased efficiency and accuracy compared to state-of-the-art approaches when applied to synthetic examples with unimodal and multimodal posteriors, ranging from low to moderate dimensionality.

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CP13

Sequential Design for Gaussian Process Surrogate Modeling in Bayesian Inverse Problems

Sequential design is a dynamic field of research in active learning whose goal is to find design strategies for costly computer models to make the most of a low computational budget. It is widely used in uncertainty quantification to build efficient surrogate models of complex computer codes. Other applications in Bayesian optimization and importance sampling have also been thoroughly investigated. This work proposes a new sequential design strategy for Gaussian Process (GP) surrogate modeling in Bayesian inverse problems. The foundation of this method is the Stepwise Uncertainty Reduction (SUR) paradigm, in which new design points are chosen sequentially by minimization of the expectation of a given metric of uncertainty. Our sequential design strategy is derived from I-optimal criterion designs and minimizes the weighted integrated predictive variance of the surrogate model, which acts as the metric of uncertainty. For GP surrogate models, the tractability of this approach is proven and a theoretical guarantee of the almost sure convergence is derived for the integrated variance. This strategy is applied to a variety of academic test cases and a practical test case in stochastic neutronics and it is compared to other (D-)optimal designs.

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CP14

Multiscale Data-Driven Model Discovery with Coherent Spatio-Temporal Scale Separation (costs)

Coherent spatiotemporal scale separation (COSTS) is a powerful scale separation method that refines the multiresolution dynamic mode decomposition (mrDMD). For each decomposition level, a DMD model is recursively fit to windows of the data, removing the slowest evolving frequency band before progressing to the next level. Upon completion of the recursive scale separation, a global scale separation is performed, yielding distinct frequency bands and their associated coherent spatial structures. As a result COSTS can describe data with complex multiscale and non-stationary features. In this talk we demonstrate how COSTS addresses two long-standing questions in geo-

physics: 1) gravity waves in observations and 2) grey zone turbulence in numerical weather models. Both sets of problems are characterized by complex interactions between multi-scale features which defy analytical solutions while also having substantial societal impacts e.g. by informing weather model performance. In the first case, non-monochromatic gravity waves are successfully characterized for the first time ever. In the second case, we can explicitly describe the spatiotemporal processes present in the grey zone, which is also a major breakthrough. Through these results we demonstrate the powerful potential of COSTS through its combination of scale separation with data-driven model discovery.

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CP15

Rare Event Estimation of Reinforcement Learning Models

Despite the rapid growth of autonomous systems and their integration into real-world applications, their accurate assessment of their accuracy and efficacy remains challenging due to high dimensionality of external uncertainty, model error, and mix of discrete and continuous variables. Consequently, the uncertainty analysis of models of autonomous systems remains untenable for most settings. In this work, we adapt rare event estimation methods to models of autonomous systems. We construct novel combinations of extreme value theory and dynamic importance sampling methods that are able to accurately estimate the failure probability of reinforcement learning models by constructing biased actions. We show that the approach is also able to discover intentionally poisoned reinforcement learning models with hidden modalities of failures.

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CP15

Uncertainty Quantification in Coastal Aquifers Using the Multi-Level Monte Carlo Method

We are solving a problem of salinisation of coastal aquifers. As a test case example, we consider the Henry salt-water intrusion problem. Since porosity, permeability and recharge are unknown or only known at a few points, we model them using random fields and random variables. The Henry problem describes a miscible two-phase flow and is nonlinear and time dependent. The solution to be found is the expectation of the salt mass fraction, which is uncertain and time-dependent. To estimate this expectation, we use the well-known multilevel Monte Carlo (MLMC) method. The MLMC method takes just a few samples on computation-ally expensive (fine) meshes and more samples on cheap (coarse) meshes. Then by building a telescoping sum, the MLMC method estimates the expected value at a much lower computational cost than the classical Monte Carlo method. The deterministic solver used here is the well-known parallel and scalable UG4 solver

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CP16

Enhancing Multi-Objective Bayesian Optimization with Learning Curves

Many real-world applications, such as training machine learning models or monitoring the effect of drug designs, involve inherently uncertain and time-consuming learning procedures. These procedures allow one to iteratively observe the performance of a solution over time, leading to the generation of learning curve. Therefore, by early stopping the learning procedures for solutions that may yield poor performance, recent studies exploited the learning curves to improve the efficiency of identifying the optimal solution under uncertainty. However, the insights offered by these learning curves are typically under-exploited in multi-objective contexts. In this study, we propose for the first time to integrate the learning curves into multi-objective optimization and reveal the optimal trade-offs on the learning curves that were overlooked by the earlier studies. We further present a new Bayesian optimization algorithm that assesses a solution based on the expected improvement of its predictive learning curves and tracks the iterative learning procedure for early stopping. Numerical experi-

ments on diverse hyperparameter tuning benchmarks indicate that our algorithm outperforms the state-of-the-art multi-objective optimizers, both in locating better trade-offs and in tuning efficiency.

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CP16

A New Approach to Null Proportion Estimation in Large-Scale Simultaneous Hypothesis Testing

We present a new approach for estimating the proportion of null effects, a vital yet difficult problem associated with large-scale simultaneous hypothesis testing. Our approach utilizes naturally nonparametric mixtures and makes a novel use of a profile likelihood function. Computational methods will also be described. Numerical studies show that the new estimator has an apparently convergent trend and outperforms the existing ones in the literature in various scenarios.

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CP16

Model Calibration and Selection for Beryllium Strength

Metal strength models rely on physical mechanisms and calibrated parameters to predict the stress response at a variety of experimental conditions. Model forms must balance theorized physics, fidelity to experimental data, and computational expense. A newly proposed strength model for hexagonal close-packed (HCP) crystal structures characterizes flow stress based on competition between deformation mechanisms–namely, twinning and slip. Strength data for the HCP metal beryllium (Be) were collected in Kolsky bar and quasistatic experiments at a variety of strain rate and temperature conditions. We use a hierarchical Bayesian model to fit the slip-twinning model, as well as several common competitors, to the Be data. We further explore the impact of modeling choices, including the applicable experimental domain and the error structure. Model selection is performed via Bayesian cross validation, which prioritizes generalization to unseen data and untried experimental conditions.

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CP16

Adaptive Importance Sampling for Deep Ritz

We introduce an adaptive sampling method for Deep Ritz method aimed at solving partial differential equations (PDEs). Two deep neural networks are used in our method. One network is employed for approximating the solution of PDEs, while the other is a deep generative model used to generate new collocation points for refining the training set. The adaptive sampling procedure consists of two main steps. The first step is solving the PDEs using Deep Ritz method by minimizing an associated variational loss on the collocation points in the training set. The second step involves generating a new training set, which is then used in subsequent computations to further improve the accuracy of the current approximate solution. We treat the absolute value of integrand in the variational loss as a probability density function (PDF) and approximate it using a deep generative model called bounded KRnet. The new samples and their associated PDF values are obtained from the bounded KRnet. With these new samples and their associated PDF values, the variational loss can be approximated more accurately using importance sampling. The proposed adaptive method can improve accuracy, particularly for problems characterized by low regularity and high dimensionality when compared to the original Deep Ritz method. We demonstrate the effectiveness of our new method through a series of numerical experiments.

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CP17

A Transformer Surrogate for Modeling the Response of Flexible Structures Submitted to Vortex-Induced Vibrations

The accurate prediction of structural instability caused by vortex shedding behind bodies or by nonlinear unsteady aerodynamics is fundamental to avoiding the degradation of structural performance or even failure of the system. Numerous approaches can represent analytical models to model both the structure and fluid. The CFD (Computational Fluid Dynamics) approach consists of solving the

Navier-Stokes equations directly, mostly limited by heavy computational costs that, many times, are tough to satisfy in practical engineering. To increase the expectations of solving practical problems, surrogate models are an alternative approach to the underlying physics. Such models have become an essential tool to simplify the analysis and can be a very useful tool in broad industrial applications. In this work, we propose the self-attention transformers model to act as a surrogate for vortex-induced vibrations (VIV) dynamics. We show by numerical experimentation that the surrogate model can accurately predict the VIV dynamics, and more importantly, it can be a suitable tool for many-query applications like sensitivity analysis, design, optimization, or uncertainty quantification.

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CP17

Analysis and Computation of a Stochastic Cahn-Hilliard System Modeling Tumor Growth

We present a system of SPDEs, which models tumor growth with stochasticity, chemotaxis, and active transport. The stochasticity of the system is modelled by random initial data and space-time white noise that appears on the right-hand side of the tumor and nutrient equations. The volume fraction of the tumor is governed by a stochastic phase-field equation of Cahn-Hilliard type, and the mass density of the nutrients is modelled by a stochastic reaction-diffusion equation. We prove the existence of a probabilistic weak solution via approximation arguments and appropriate compactness theorems. Lastly, we propose a numerical approximation based on the Galerkin finite element method in space and the semi-implicit Euler-Maruyama scheme in time. We illustrate the effects of the stochastic components in the tumor growth by some numerical simulations.

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CP17

Unbiased Estimation for Wright-Fisher Diffusion Processes: An Exact Simulation Approach

In this talk I will present an unbiased Monte Carlo maximum likelihood estimator for discretely observed Wright-Fisher diffusions. Our approach is based on exact simulation techniques that are of special interest for diffusion processes defined on a bounded domain, where numerical methods typically fail to remain within the required boundaries. We start by building unbiased maximum likelihood estimators for scalar diffusions and later present an extension to the multidimensional case. Consistency results of our proposed estimator are also presented and the performance of our method will be illustrated through numerical examples.

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CP17

Uncertainty Quantification and Global Sensitivity Analysis of Seismic Fragility Curves Using Kriging

Seismic fragility curves have been introduced as key components of Seismic Probabilistic Risk Assessment studies. They express the probability of failure of mechanical structures conditional to a seismic intensity measure and must take into account the inherent uncertainties in such studies, the so-called epistemic uncertainties (i.e. coming from the uncertainty on the mechanical parameters of the structure) and the aleatory uncertainties (i.e. coming from the randomness of the seismic ground motions). For simulation-based approaches we propose a methodology to build and calibrate a Gaussian process surrogate model to estimate a family of non-parametric seismic fragility curves for a mechanical structure by propagating both the surrogate model uncertainty and the epistemic ones. Gaussian processes have indeed the main advantage to propose both a predictor and an assessment of the uncertainty of its predictions. In addition, we extend this methodology to sensitivity analysis. Global sensitivity indices such as aggregated Sobol indices and kernel-based indices are proposed to know how the uncertainty on the seismic fragility curves is apportioned according to each uncertain mechanical parameter. This comprehensive Uncertainty Quantification framework is finally applied to an industrial test case consisting in a part of a piping system of a Pressurized Water Reactor. The preprint associated to this work is available at the following URL: https://arxiv.org/abs/2210.06266

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CP18

Weighted Leave-One-Out Cross Validation

We present a weighted version of Leave-One-Out (LOO) cross-validation for estimating the Integrated Squared Error (ISE) when approximating an unknown function by a predictor that depends linearly on evaluations of the function over a finite collection of sites. The method relies on the construction of the best linear estimator of the squared prediction error at an arbitrary unsampled site based on squared LOO errors, assuming that the function is a realization of a Gaussian Process (GP). A theoretical analysis of performance of the ISE estimator is presented, and robustness with respect to the choice of the GP kernel is investigated first analytically, then through numerical ex-

amples. Overall, the estimation of ISE is significantly more precise than with classical, unweighted, LOO cross validation. Application to model selection is briefly considered through examples.

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CP18

Deep Priors in a Probabilistic Full Waveform Inversion

Estimating the subsurface velocity field is a critical piece within the decision chain in the oil industry. Therefore, there is a need to provide reliable evaluations of uncertainties due to the limitations (noisy measurements, model discrepancies, and sparse data) of the inversion process. Here, we present a probabilistic formulation relying on using, as a prior for the Bayesian inference, Convolutional Neural Networks for parameterizing the velocity field. Indeed, assuming the configuration of a generative model, the hyperparameters of the neural network become the target of the inversion. The numerical results demonstrate the regularization effect promoted by such a choice. The likelihood is formed assuming Gaussian noise at the seismic sensors and the wave elastic equations as the forward model. Finally, the posterior probability distribution samples are computed using a stochastic gradient Langevin algorithm. Some examples employing synthetic data are used to illustrate the overall performance of the proposed formulation.

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CP18

Design of a Proper and Objective Bayesian Methodology to Estimate Seismic Fragility Curves

Seismic fragility curves are key quantities of the Seismic Probabilistic Risk Assessment studies carried out on industrial facilities. They express the probability of failure of a mechanical structure conditional to a scalar value derived from the seismic ground motion called Intensity Measure (IM). Estimating such curves is a daunting task because for most structures of interest few data are available. For this reason, a wide range of the methods of the literature rely on a parametric log-normal model. The Bayesian approach permits an efficient learning of the parameter which determine the fragility curves. It avoids the generation of unrealistic samples, which are common with classical methods. We enrich the reference prior theory to question the prior selection. Our work supports the implementation of the Jeffreys prior which we derive for this problem. Our results prove the superiority and the robustness of this prior over the ones of the literature. Also, they unveil how the distribution of the observed data might lead to phenomena that we defined as degenerate, and which can lead to improper posteriors. We verify those phenomena to be more likely to happen when the number of observations is low or when the considered IM is more correlated to the structure response. Our conclusions are published in an arXiv preprint (arXiv:2302.06935).

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CP19

Uncertainty Quantification for Anomaly Detection in Wearable Health Data

Considering the recent pandemic, early detection of new outbreaks is critical for deploying timely intervention. We developed and applied advanced anomaly detection methods for health datasets collected from wearable datasets at multiple resolutions of population (individual to population). We utilize this strategy for early detection of infection in individuals timelines and outbreak hotspots in a population. To achieve this, we need a real-world health physiological dataset from wearables (heart rate, activity, temperature, etc.) for a population experiencing an infectious outbreak to train and evaluate anomaly detection methods. Although some data is available for individuals and populations for the recent pandemic, significant data gaps hinder the development of integrated multilayer anomaly detection. We utilize Generative Adversarial Networks (GANs) to generate real-world-inspired wearable data for a population in an infectious outbreak. We use these synthetic datasets to employ a co-kurtosis-based projection pursuit technique to detect anomalies within multivariate time-series data. Further, we comprehensively assess uncertainties in synthetic data vs. its real-world counterparts and uncertainty associated with fine-tuning the threshold for detecting anomalies in physiological measurements. We demonstrate an improved method for early detection of abnormalities in multivariate datasets and promising applications in healthcare and beyond.

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CP19

Learning and Interpolating Continuous Empirical Green's Functions

In this work, we present a mesh-independent, data-driven approach to mathematically model one-dimensional systems, possessing an associated control parameter (θ), and whose governing partial differential equation is *unknown*. The proposed method learns a *Empirical* Green's Function for the associated, but hidden, boundary value problem

($\mathcal{L}_\theta u(x) = f(x), \forall x \in \Omega \subset \mathbb{R}$). The subject system is observed by collecting input-output pairs of system responses (outputs) at different control parameter values, under excitations (inputs) that are drawn from a Gaussian process. We learn a Green's function, for each control parameter value, in the form of a Rational Neural Network [Boull N. et al., Sci Rep 12, 4824, 2022] and then represent these in terms of a continuous singular value expansion, using our python implementation of the Chebfun library [Driscoll T. A. et al., Chebfun Guide, Pafnuty Publications, 2014]. We uncover the Green's function, at an unseen control parameter value, by interpolating the left and right singular functions within a suitable *library*, expressed as points on a manifold of *Quasimatrices* ($(L^2(\Omega))^K$), while the associated singular values are interpolated with Lagrange polynomials. The approximation and interpolation numerical techniques are demonstrated on several examples.

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CP19

Dimension Reduction for Uncertainty Propagation and Global Sensitivity Analyses in a Sequence of Models

This talk presents an efficient method to perform uncertainty propagation in a calculation chain made up of two numerical models, namely a cesium adsorption model upstream chained with a pore water composition model. As the number of uncertain input parameters is about twenty for each of the two models, a dimension reduction technique is implemented to build a polynomial approximation of the QoI in a reduced subspace. Two approaches are tested depending on the two models are treated as a single block or two separate blocks. We observe that the interpretation of the linear transformations projecting the original inputs to the reduced coordinates is broadly consistent with the geochemical features of the model. Validation results show that the relative error levels of the surrogate models are around a few percent for both approaches with only one thousand realizations of the chained model. Global sensitivity analysis highlights that the variance of the QoI is overwhelmingly governed by the adsorption model. This conclusion is nuanced when considering the whole cumulative distribution function for which the interaction effects between the two models account for a fifth.

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CP20

Tackling the Curse of Dimensionality: A Generative Modeling Approach to Linear Response Theory

In many applications, particularly turbulent atmospheric and oceanic systems, finding the optimal response is essential but challenging due to their complexity. The Fluctuation-Dissipation Theorem (FDT) facilitates gauging system response via current state statistics, benefiting climate science by reducing computational demands. It's been effective in General Circulation Models (GCMs) and applied in areas like sea surface temperature and turbulence modeling. Implementing FDT requires estimating the gradient of the system's equilibrium probability distribution function (PDF), which is difficult in high-dimensional systems due to the "curse of dimensionality." The quasi-Gaussian (qG) method, which uses a Gaussian approximation for the equilibrium PDF, is popular but can introduce biases in situations with strong non-Gaussian features. This study utilizes generative modeling techniques to construct the gradient. Generative modeling transforms complex data distributions into known prior distributions, with a reverse-time SDE restoring the original distribution using its gradient field, determined by neural networks.

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CP20

Differential Contagiousness of Respiratory Disease Across the United States

The initial contagiousness of a communicable disease within a given population is quantified by the basic reproduction number, $\mathcal{R}_0$. This number depends on both pathogen and population properties. On the basis of compartmental models that reproduce Coronavirus Disease 2019 (COVID-19) surveillance data, we used Bayesian inference with uncertainty quantification and the next-generation matrix approach to estimate region-specific values for 280 of 384 metropolitan statistical areas (MSAs) in the United States (US), which account for 95% of the US population living in urban areas and 82% of the total population. We focused on MSA populations after finding that these populations were more uniformly impacted by COVID-19 than state populations. Our maximum a posteriori (MAP) estimates for $\mathcal{R}_0$ range from 1.9 to 7.7 and quantify the relative susceptibilities of regional populations to spread of respiratory diseases.

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CP20

A Matrix Splitting Approach for Kalman Filtering on Partially Unknown Models

Partially unknown models arise frequently in Kalman filtering, e.g. when the filter state is augmented to describe the dynamics of an unknown input or when a subsystem is modelled roughly. Typically, it results that the model matrix has a principal submatrix less precise than the remaining part. In this talk we present a novel Kalman Filter formulation that gives practical advantages when the more and the less precise parts of the model matrix can be additively splitted satisfying a few properties. If it holds, this Splitting Kalman Filter (SKF) shows lower influence from matrix ill-conditioning and less computational effort in a wide range of conditions. For this reason, it becomes a good choice e.g. for methods that propagate an ensemble of models, like it is done in recent trends in sparse, data-driven modelling of dynamical systems, and in well-known sample-and-propagate methods, where it is needed to propagate a set of representative samples of the estimated distribution. We show some results from a simultaneous estimation of temperatures and heat flux in a heat transfer model problem.

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CP20

Hidden Crash Constraints Management for the Robust Design Optimization of Wind Turbines

The robust design optimization of wind turbines generally requires numerous computationally expensive code simulations with different sets of values of both design variables and environmental wind load variables. However, the simulators encounter simulation crashes due to convergence issues for some values of both input variables. These failures correspond to a hidden constraint and might be as costly to evaluate as a feasible simulation. The presence of such crashes must be managed in a wise way during the robust optimization computation, in order to target feasible input areas and thus avoid unnecessary irrelevant simulations. In this context, three different objectives will be addressed for a wind turbine reliable design application: (i) the active learning of the hidden constraint, then (ii) its coupling with a sequential space-filling design to obtain a metamodel of the damage on the structure and (iii) its coupling with an optimization procedure for designing a reliable wind turbine with a minimal weight.

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MS1

A Reduced Basis Sampling Strategy for Problems with High-Dimensional Parameters

In the last two decades, model order reduction has been established as an important tool for the solution of high-dimensional parametrized partial differential equations. However, even with the development and success of new methods that exploit machine learning tools, the problem of offline sampling remains. Most methods still rely on a random sampling of the parameter space, which especially in high-dimensional parameter spaces necessitates large amounts of training data. We explain a novel method to determine where to sample, therefore reducing the number of samples required. Our method, the Polytope Dimension scheme, significantly reduces the computation time to construct a reduced basis in higher dimensions while maintaining errors of the same order of magnitude.

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MS1

State Estimation with Wasserstein Reduced Models

In this work, we are concerned with the problem of optimal recovery of solution states to convection-dominated parametrized PDEs posed on the 2-Wasserstein space, through finitely many observations. To this end, we, first, reduce the complexity of the problem by approximating the parametric PDE solution manifold through a n-dimensional nonlinear space generated by a set of Wasserstein barycenters (Cohen et al., Anal. Appl., 21 (2023), pp. 217-253; Ehrlacher et al. Math. Model. Numer. Anal., 54 (2020), pp. 21592197). This allows for a collective estimation of the elements of the solution manifold. We, then, design a recovery algorithm, based on barycenters, that recovers the solution states from the data collected through a set of sensors, in the form of linear functional evaluations. The performance of the recovery algorithm relies on a *stability* constant and the worst case error attained when approximating the solution manifold. Here, the stability constant depends implicitly on the sensor location. We, therefore, optimize over the sensor locations and provide bounds on the stability constant to ensure a reliable recovery of the solution state. Finally, we validate our algorithm for robustness against several parametric PDEs such as the Burgers, the Camassa-Holm, the KDV and the Vlassov-Poisson equations.

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MS1

Generating Reduced Order Models Parallel in Time via Random Sampling

To tackle time-dependent partial differential equations (PDEs) with coefficients that are rough in both space and time, we construct reduced basis functions defined in space that can be combined with time stepping schemes, e.g., within model order reduction methods. As a key new contribution, we propose to construct these ansatz functions in an embarrassingly parallel and local manner in time by

selecting important points in time and only performing local computations on the corresponding local time intervals. [Schleu, Smetana, ter Maat, 2023] In detail, we perform several simulations of the PDE for only few time steps in parallel, starting at different, randomly drawn start time points, prescribing random initial conditions. Applying a singular value decomposition to a subset of the so obtained snapshots yields the reduced basis functions. To select suitable start points in time, we suggest using data-driven sampling strategies from randomized numerical linear algebra such as leverage score sampling. By solving the PDE locally in time with random initial conditions, we construct local ansatz spaces in time that converge provably at a quasi-optimal rate and allow for local error control. Numerical experiments demonstrate that the proposed approach can outperform existing methods like the proper orthogonal decomposition even in a sequential setting and is well capable of approximating advection-dominated problems.

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MS1

Weighted Reduced Order Methods for Nonuniformly Distributed Parameters: a Collection of Methods

In numerous optimization scenarios and uncertainty quantification tasks, the necessity arises to address stochastic partial differential equations (PDEs). In these instances, stochasticity impacts various parameters of the PDE, including forcing terms, equation coefficients, boundary conditions, and initial conditions. We assume knowledge of the probability distribution underlying these parameters. Hence, we take advantage of the resulting parametrized formulation to propose an efficient reduced order model. Additionally, we exploit the inherent stochastic assumption to define appropriate weights that guide the reduction process. Three viable strategies are discussed: the weighted reduced basis method, the weighted proper orthogonal decomposition method and the weighted convolutional neural network. The proposed methodologies are illustrated through a selection of numerical examples.

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MS2

Multi-fidelity Methods for a Class of Kinetic Models with Uncertainties

In this talk, we will discuss some recent development on multi-fidelity methods for solving a class of kinetic models with uncertainties and multiple scales. The Boltzmann equation, linear transport equation, Vlasov-Poisson equation, semi-classical Schrdinger equation and epidemic transport system will be studied. We will provide some formal error analysis. Many simulations will be presented to justify the robustness and accuracy of the numerical schemes. These are joint work with Lorenzo Pareschi,Xueyu Zhu and Guilia Bertaglia.

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MS2

Stochastic Galerkin Particle Methods for Kinetic Equations of Plasmas with Uncertainties

The study of plasma models is receiving a great deal of attention from the scientific community because of its potential applications to nuclear fusion reactors. At the kinetic scale, the time evolution of the distribution functions in plasmas is described by the Landau equation. Besides, the importance of considering uncertainties in such equations has been recognised. The inclusion of random parameters poses additional challenges. From an analytical point of view, it is crucial to study the dependence of the solution on the parameter in order to guarantee the regularity of the model. This is also important for the construction of numerical methods, which must deal with the natural increase in the dimensionality of the equation, typically known as the curse of dimensionality. Recently, a new class of numerical methods that combine a particle-based approximation of the distribution function in the phase space together with a stochastic Galerkin expansion of the particles in the random space has been proposed [1,2]. [1] A. Medaglia, L. Pareschi, M. Zanella, *Particle simulation methods for the Landau-Fokker-Planck equation with uncertain datas*, arXiv preprint arXiv:2306.07701, 2023. [2] A. Medaglia, L. Pareschi, M. Zanella, *Stochastic Galerkin particle methods for kinetic equations of plasmas with uncertainties*, Journal of Computational Physics, 479 (2023), pp. 112011.

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MS2

Applications of UQ in Accident Traffic Models

We study an accident traffic model given by a hyperbolic partial differential equation with a space-dependent flux function. The spatial dependence arises from the choice of uncertain accident parameters, such as accident position or accident severity, which introduce additional uncertainty into the flux function. Assuming data-based probability distributions for the accident parameters, we numerically investigate expectations and quantiles of traffic densities. In addition, we set up an inverse problem to reobtain information about the accident parameters based on observations of traffic densities.

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MS2

Efficient Inference for Bayesian Physics Informed Neural Network

Bayesian Physics Informed Neural Networks (B-PINNs) have gained significant attention for PDE-based inverse problems. Existing inference approaches are either computationally expensive for high-dimensional posterior inference or provide unsatisfactory uncertainty estimates. In this paper, we present a new efficient inference algorithm for B-PINNs that uses Ensemble Kalman Inversion (EKI). We find that our proposed method can achieve inference results with informative uncertainty estimates comparable to Hamiltonian Monte Carlo (HMC)-based B-PINNs with a much reduced computational cost.

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MS3

Uncertainty Quantification for Endocrine State and Phenotype Forecasting in the ICU

Precision medicine strategies traditionally rely on omics data to identify discrete disease subtypes and then develop and tailor treatments based on membership to a given phenotype. When disease and treatment are discrete, this discrete phenotypic model for understanding physiology and choosing intervention is highly effective. However, in many situations physiological states more accurately represented as a collection of processes that vary continuously. One example of such a situation is the endocrine system of patients in an intensive care unit (ICU). In these situations, it can be useful to model for forecast the system with mechanistic physiological models to both further our understanding of physiological mechanics and use this understanding to tailor treatment to an individual patients current state. Here we focus on managing model and forecast uncertainty present in both continuous state and phenotypic forecasting in an ICU setting. Within this context we define forecasting pipelines, consider model, and forecast uncertainty roadblocks, and discuss recent progress as it generalizes to many other physiological settings.

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MS3

A Reproducible Bayesian Workflow for Processing Highly Heterogeneous Time Resolved Medical Data

Living systems can show significant variability. In a medical context, this variability is in addition overlayed by inter-individual differences like age, weight, gender or lifestyle of a patient, leading to high variances between replicates in time series measurements in longitudinal studies, and even more in cross-sectional studies. Bayesian approaches are frequently used to quantify uncertainties in these settings. We introduce BayModTS (Bayesian Modeling of Time Series Data), a Bayesian workflow for analyzing heterogeneous time-resolved medical data. In BayModTS, posterior distributions are investigated by sampling from a dynamical model. Posterior predictive distributions and summary statistics like credibility intervals thereof quantify the respective uncertainty in model predictions. We show the results of BayModTS for two different application scenarios within our research unit FOR 5151 QuaLiPerF (Quantifying Liver Perfusion-Function Relationship in Complex Resection): 1. In cooperation with Prof. Uta Dahmen and Mohamed Albadry (University Hospital Jena), we use BayModTS to investigate differences in the metabolization of drugs in mice subject to feeding different fat diets. 2. Taking clinical liver volumetry data from Prof. Michael Tautenhahn and Eva Kindler (University Hospital Leipzig), we apply BayModTS to characterize liver regeneration courses of male and female patients after liver resection.

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MS3

Building a Random Forest Pipeline to Aid the Non-Invasive Scoring of Fibrosis in NAFLD

Non-alcoholic steatohepatitis (NASH), the severe form of non-alcoholic fatty liver disease (NAFLD) is becoming a growing global health concern characterized by liver fat build-up, inflammation, cellular damage, and fibrosis. The fibrosis stage, determined invasively by liver biopsy, is the primary predictor of disease progression and prognosis. While FIB-4 is a common non-invasive clinical index, its reliance on two thresholds leaves about 30% of patients unclassified, underscoring the need for an improved fibrosis diagnostic model to guide clinical evaluation and management. We studied a NAFLD clinical cohort (87 patients) with data for more than 1000 biomarkers. Due to the datas high dimensionality, we developed a random forest pipeline aimed to extract biomarkers linked to fibrosis. First, we used the Boruta feature selection aiming to select "all-relevant" features. Second, we ran a range of random forest models based on different subsets of biomark-

ers. Nested cross-validation showed the Boruta selection consistently outperformed all other models employing approximately 20–40 biomarkers. This random forest model showed high accuracy (AUROC 0.90, Accuracy 0.85) and low misclassification, similarly to the FIB-4 score (AUROC 0.80, Accuracy 0.88), whilst allowing for the classification of all patients. These results indicate that random forest models enhance non-invasive fibrosis assessments, enabling their application in clinical trials and patient risk stratification.

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MS3

A Fully Hierarchical Bayesian Approach to Sequentially Update Population Parameter Uncertainty in Model-Informed Precision Dosing

In model-informed precision dosing, mathematical models are used to predict therapy outcomes by combining prior information, patient characteristics, and patient-specific measurements. Prior information, the population parameter estimates are derived from a clinical study population. As additional data from individuals in clinical treatment becomes available, an update of the prior information is reasonable to appropriately represent the target population and correct potential parameter bias. To this end, we propose a sequential hierarchical Bayesian approach based on [Corinna Maier et al., 2022] and [Nicolas Chopin et al., 2013] that supports the representation of uncertainty in our prior information via the use of a hyperprior and a sequential update thereof. With this two-level nested particle filter, data is first assimilated on the individual level to update the individual priority. In the second step, the individual posterior is then used to update the hyperprior. By assimilating data sequentially, we do not require sensitive patient measurements to be stored beyond the course of treatment. Instead, an immediate update of the hyperprior, which then contains all relevant information, is performed. The nested approach was tested against a non-sequential hierarchical MCMC method in a simple model system. It has shown comparable approximation performance with both dense and sparse data available per individual.

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MS4

A New Operator-Theoretic Formulation and Algorithm for Transport-Based Bayesian Inference

In the fully Bayesian setting, such as in Bayesian data assimilation and inverse problems, we are interested in sampling from high-dimensional and often non-Gaussian and complex Bayesian posteriors. Often, the target distribution is available up to a normalization constant, which means that the score of the distribution, defined as the logarithm of the gradient of its density, is known. Here we present a new iterative transport-based methodology that uses the score to generate samples from the target. Specifically, we develop a Newton method designed to find the transport map as the zero of a "score-residual' operator. This infinite-dimensional transport algorithm is particularly inspired by the setting of Bayesian filtering. When the underlying dynamical system is chaotic, the target posteriors are singular but have an underlying structure that can be exploited for a fast and accurate estimation of their conditional scores. The constructed transport map hence allows for provably consistent sampling that exploits low-dimensional structure in the target.

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MS4

Spatiotemporal Statistical Modelling with Stochastic PDEs

Most environmental data sets contain measurements collected over space and time. It is the purpose of spatiotemporal statistical models to adequately describe the underlying uncertain spatially explicit phenomena evolving over time. In this talk I will present a new class of spatiotemporal statistical models which is based on stochastic partial differential equations (SPDEs) involving fractional powers of parabolic operators. In particular, I will discuss the efficient simulation of the spatiotemporal solution processes, which is closely related to the approximation of nonlocal space-time differential operators. Furthermore, I will address the motivation for employing this class of SPDEs in statistical applications and give an outlook on the computational benefits for statistical inference from spatiotemporal data.

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MS4

Subsampling Error in Stochastic Gradient Langevin Diffusion

The Stochastic Gradient Langevin Dynamics (SGLD) are popularly used to approximate Bayesian posterior distributions in statistical learning procedures with large-scale data. As opposed to many usual Markov chain Monte Carlo (MCMC) algorithms, SGLD is not stationary with respect to the posterior distribution; two sources of error appear: The first error is introduced by an Euler–Maruyama discretisation of a Langevin diffusion process, the second error comes from the data subsampling that enables its use in large-scale data settings. In this work, we consider an idealised version of SGLD to analyse the method's pure subsampling error that we then see as a best-case error for diffusion-based subsampling MCMC methods. Indeed, we introduce and study the Stochastic Gradient Langevin Diffusion (SGLDiff), a continuous-time Markov process that follows the Langevin diffusion corresponding to a data subset and switches this data subset after exponential waiting times. There, we show that the Wasserstein distance between the posterior and the limiting distribution of SGLDiff is bounded above by a fractional power of the mean waiting time. Importantly, this fractional power does not depend on the dimension of the state space. We bring our results into context with other

analyses of SGLD.

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MS4

Experimental Design for Gaussian Process Regression in High-Dimensional Inverse Problems

Bayesian posterior distributions arising in modern applications are often computationally intractable due to the large computational cost of evaluating the data likelihood. Examples include inverse problems in partial differential equation models arising in climate modeling and in subsurface fluid flow. To alleviate the problem of expensive likelihood evaluation, a natural approach is to use Gaussian process regression to build a surrogate model for the likelihood, resulting in an approximate posterior distribution that is amenable to computations in practice. In this talk, we present new insights into a suitable choice of training points in this context. We show that the error between the true and approximate posterior distribution can be bounded by the error between the true and approximate likelihood, measured in the ??2-norm weighted by the true posterior; furthermore we show that minimizing the error between the true and approximate likelihood in this norm suggests choosing the training points in the Gaussian process surrogate model based on the true posterior.

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MS5

Fredholm Integral Equations for the Training of Shallow Neural Networks

We present a novel approach for the training of single-hidden-layer neural networks, based on the approximate solution of associated Fredholm integral equations of the 1. kind by Ritz-Galerkin methods. We show how tensor decompositions and Tikhonov regularization can be used to construct continuous counterparts of discrete neural networks with an infinitely large hidden layer. The efficiency and reliability of the introduced approach is illustrated by the practical application to several supervised learning problems.

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MS5

Low-rank Tensor Approximation of High-Dimensional Functions

In this talk, we analyze tensor approximation schemes for high-dimensional functions in the continuous setting. To this end, we assume that the function to be approximated lies either in an isotropic Sobolev space or an anisotropic Sobolev space. We apply successively the truncated singular value decomposition in order to discuss the cost when approximating the function under consideration in the continuous analogues of tensor formats such as the Tucker tensor format or the tensor train format. Special attention is paid on the situation that dimension weights appear.

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MS5

Optimal Sampling for Approximate Gradient Descent

Approximating high-dimensional functions often requires optimising a loss functional that can be represented as an expected value. When computing this expectation is unfeasible, a common approach is to replace the exact loss with a Monte Carlo estimate before employing a standard gradient descent scheme. This results in the well-known stochastic gradient descent method. However, using an estimated loss instead of the true loss can result in a "generalisation error". Rigorous bounds for this error usually require strong compactness and Lipschitz continuity assumptions while providing a very slow decay with increasing sample size. This slow decay is unfavourable in settings where high accuracy is required or sample creation is costly. To address this issue, we propose a new approach that involves empirically (quasi-)projecting the gradient of the true loss onto local linearisations of the model class through an optimal weighted least squares method. The resulting optimisation scheme converges almost surely to a stationary point of the true loss, and we investigate its convergence rate.

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MS6

Tensor Train Approximation of PDE Solution Maps

PDE inverse problems suffer from vast computational complexity due to the need to solve an already numerically expensive PDE many times on samples of random variables (parameters) in the Bayesian inference, or iterations of an optimisation method in the deterministic formulation. Moreover, full PDE solutions don't incorporate any regularisations (such as smoothness), and can be less accurate if a noisy input is given. In this talk we propose to pre-compute a surrogate coefficient-to-solution map using the Tensor Train (TT) decomposition. Firstly, random fields representing PDE coefficients are approximated in a finite-dimensional linear basis with the dimensions ordered by importance. Secondly, the PDE solution as a function of finite-dimensional parameters of the coefficient is approximated in the TT format. This step uses the ALS-Cross approximation method to solve the PDE non-intrusively on adaptively chosen samples of the parameters. Finally, a linear output of the solution can be encoded into the same TT decomposition. We show that the TT approximation of the solution can significantly speedup sampling in Bayesian inverse problems constrained by elliptic and elasticity PDEs.

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MS6

An Operator Network Architecture for Functional SDE Representations

Deep Operator Networks (DON) represent a Neural Network architecture that is amenable to a complete convergence analysis by splitting the occurring approximation error into accessible stochastic and deterministic components. It has been shown that the trunk and branch structure can be exploited in the framework of polynomial chaos expansions (PCE) for solutions of parametric PDE as they are thoroughly examined in the field of uncertainty quantification. In this talk, we are concerned with stochastic differential equations (SDE) for which it is rather uncommon to pursue a functional representation, in particular when performing numerical computations. A main reason is the high complexity due to the exponential growth of a polynomial basis in the dimension of the problem and the degree. This approach only becomes amenable in practice if some form of compression of the basis can be relied upon, which e.g may be achieved by using modern approximation techniques such as Neural Networks or hierarchical Tensor Networks. We present a complete error analysis of the PCE of SDE solutions with an adapted DON architecture and demonstrate the (favorable) practical performance with some benchmark problems. Moreover, we review some aspects of the challenging task of simulating backward SDE. Here, the PCE offers the unique advantage that conditional expectations translate to appropriate truncations, which enables efficient numerical schemes beating typical sampling methods.

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MS6

Score-Based Diffusion Models in Function Space

We present a generalization of score-based diffusion models to function space by perturbing functional data via a Gaussian process at multiple scales. We obtain an appropriate notion of score by defining densities with respect to Guassian measures and generalize denoising score matching. We then define the generative process by integrating a function-valued Langevin dynamic. We show that the corresponding discretized algorithm generates accurate samples at a fixed cost that is independent of the data discretization.

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MS6

Data-Complexity Bounds for Operator Learning

Operator learning frameworks leverage neural networks and define a methodology for the data-driven approximation of operators. How much data is necessary to learn operators in such a purely data-driven manner? In this presentation, I will report on recent work that provides first answers on this question (joint with Nik Kovachki and Hrushikesh Mhaskar). Upper and lower bounds on the data-complexity of operator learning will be discussed.

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MS7

A General Framework for Sampling Problems Based on Diffusion Models and Schrdinger Bridges

Recently, a series of papers proposed deep learning-based approaches to sample from unnormalized target densities using controlled diffusion processes. In this work, we identify these approaches as special cases of the Schrdinger bridge problem, seeking the most likely stochastic evolution between a given prior distribution and the specified target. We further generalize this framework by introducing a variational formulation based on divergences between path space measures of time-reversed diffusion processes. This abstract perspective leads to practical losses that can be optimized by gradient-based algorithms and includes previous objectives as special cases. At the same time, it allows us to consider divergences other than the reverse Kullback-Leibler divergence that is known to suffer from mode collapse. In particular, we propose the so-called log-variance loss, which exhibits favorable numerical properties and leads to significantly improved performance across all considered approaches.

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MS7

Trajectory Generation, Control, and Safety with Denoising Diffusion Probabilistic Models

We present a framework for safety-critical optimal control of physical systems based on denoising diffusion probabilistic models (DDPMs). The technology of control barrier functions (CBFs), encoding desired safety constraints, is used in combination with DDPMs to plan actions by iteratively denoising trajectories through a CBF-based guided sampling procedure. At the same time, the generated trajectories are also guided to maximize a future cumulative reward representing a specific task to be optimally executed. The proposed scheme can be seen as an offline and model-based reinforcement learning algorithm resembling in its functionalities a model-predictive control optimization scheme with receding horizon in which the selected actions lead to optimal and safe trajectories.

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MS7

GAN-DUF: Hierarchical Deep Generative Models for Design Under Free-Form Geometric Uncertainty

Deep generative models have demonstrated effectiveness in learning compact and expressive design representations that significantly improve the efficiency and solution quality in high-dimensional geometric design optimization. However, such generative-model-augmented design optimization usually does not consider the geometric variation or uncertainty introduced by manufacturing or fabrication. Past work that quantifies such uncertainty often makes simplifying assumptions on geometric variations, while the more realistic free-form uncertainty and its impact on design performance are difficult to quantify due to the high dimensionality. To address this issue, we propose a Generative Adversarial Network-based Design under Uncertainty Framework (GAN-DUF), which contains a deep generative model that simultaneously learns a compact representation of nominal designs and the conditional distributions of fabricated designs given any nominal design. This opens up new possibilities of 1) building a universal uncertainty quantification model compatible with both shape and topological designs, 2) modeling free-form geometric uncertainties without the need to make any assumptions on the distribution of geometric variability, and 3) allowing fast prediction of uncertainties for new nominal designs. We combine the proposed deep generative model with robust design optimization and demonstrate the frameworks capability of finding solutions with better post-fabrication performance.

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MS7

Bayesian Inverse Problems with Conditional Entropic Generative Adversarial Networks in Least Volume Latent Spaces

Solving inverse problems in scientific and engineering fields has long been intriguing and holds great potential for many applications, yet most techniques still struggle to address issues such as high dimensionality, nonlinearity and model uncertainty inherent in these problems. Recently, generative models such as GANs and Diffusion models have shown great potential in approximating complex high dimensional conditional distributions and have paved the way for characterizing posterior densities in Bayesian inverse problems, yet the problems high dimensionality and high nonlinearity often impedes the models training. In this talk we show how to tackle these issues with Least Volumea novel nonlinear dimension reduction methodthat can explore low dimensional spaces using suitable autoencoders that identify latent variables such that the projected training data occupies minimum volume, thus enabling efficient and accurate training of conditional generative models in the low dimensional latent spaces. We demonstrate the power of such latent conditional GANs on a variety of applications including inversion of parameters in systems of ODEs and high dimensional hydraulic conductivities in subsurface flow problems.

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MS8

ExaGeoStat: Scalable Parallel Estimation of Exact and Approximate Likelihood Functions on Large-Scale Systems

Maximum Likelihood Estimation (MLE) is a key method in Geoscience for modeling spatial and spatio-temporal data and is applicable to various machine learning algorithms. It involves creating an npt X npt covariance matrix for geospatial data, where npt reflects the number of spatial locations, variables, and time slots. The computational complexity of MLE, particularly for large datasets, is a challenge, often reaching $O((npt)^3)$. To address this, our research combines parallel processing with matrix approximation, specifically mixed precisions and tile low-rank approximations, to improve the efficiency of the MLE operation in large-scale systems. This method achieves better compression rates and faster performance while maintaining accuracy. We tested this on several high-performance computing systems, including Riken Fugaku, ORNL Summit, KAUST Shaheen-II, and HLRS HAWK, demonstrating significant performance improvements.

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MS8

A Simple, Bias-Free Approximation of Covariance Functions by the Multilevel Monte Carlo Method in the Hilbert Space Setting

We develop simple and bias-free Monte Carlo and multilevel Monte Carlo approximations to covariance functions of sufficiently regular random fields in tensor products of Hilbert spaces. We investigate approximating the covariance function by means of full tensor product approximations, and additionally derive sparse tensor product approximation variants to overcome the curse of dimensionality and yield essentially optimal complexity, i.e., up to logarithmic factors. A priori convergence and work estimates for the different variants are given and subsequently compared theoretically and numerically, where experiments for an exemplary elliptic diffusion problem validate the theoretical findings. The Hilbert space setting allows us to develop a rather simple construction of the estimators and a simple and explicit proof strategy.

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MS8

Data Sparse Multilevel Covariance Estimation in Optimal Complexity.

The classical sample covariance or Monte Carlo estimator is prohibitively expensive for many practically relevant problems, where often approximation spaces with many degrees of freedom and many samples for the estimator are needed. We propose and analyze an $\mathcal{H}^2$-based data sparse multilevel sample covariance estimator, i.e., a multilevel Monte Carlo estimator. For this purpose, we generalize the notion of asymptotically smooth kernel functions to a Gevrey type class of kernels for which we derive new variable-order $\mathcal{H}^2$-approximation rates. These variable-order $\mathcal{H}^2$-approximations can be considered as a variant of *hp*-approximations. Our multilevel sample covariance estimator then uses an approximate multilevel hierarchy of variable-order $\mathcal{H}^2$-approximations to compress the sample covariances on each level. The non-nestedness of the different levels makes the reduction to the final estimator nontrivial and we present a suitable algorithm which can handle this task in linear complexity. This allows for a data sparse multilevel estimator of Gevrey covariance kernel functions in the best possible complexity for Monte Carlo type multilevel estimators, which is quadratic. Numerical examples which estimate covariance matrices with tens of billions of entries are presented.

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MS8

An Exponential Speedup in the Rigorous Learning of Elliptic Solution Operators

The so-called "operator learning" of solution operators of partial differential equations (PDEs) from solution pairs has attracted considerable attention. Previous rigorous methods for learning elliptic PDEs required poly$(1/\epsilon)$ solution pairs to achieve an ϵ-accurate approximation of the solution operator. In the present work, we achieve an exponential improvement by proposing an algorithm that can recover the discretized solution operators of general elliptic PDEs on a d-dimensional domain to accuracy ϵ from only $\mathcal{O}\left(\log(N)\log^d(N/\epsilon)\right)$ solution pairs selected a-priori. Here, N is the number of degrees of freedom of the discrete function space. We can also approximate the continuous Green's function (in operator and Hilbert-Schmidt norm) to accuracy ϵ from $\mathcal{O}\left(\log^{1+d}\left(\epsilon^{-1}\right)\right)$ solutions of the PDE. Our method has computational cost $\mathcal{O}\left(N\log^2(N)\log^{2d}(N/\epsilon)\right)$ and returns a sparse Cholesky factor with $\mathcal{O}\left(N\log(N)\log^d(N/\epsilon)\right)$ nonzero entries. We provide numerical experiments that show the practical performance of our method, including on fractional-order PDEs. Finally, we present applications to closure modeling in turbulent flows obtained in joint work with Spencer Bryngelson, Jessie Liu, and Ali Mani.

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MS9

Sensitivity-Based Uncertainty Quantification for Particle Monte Carlo Simulations of Neutrals in Nuclear Fusion Reactors

Plasma edge simulations are extensively used for the design of future nuclear fusion reactors and the design and interpretation of current-day experiments. The large number of uncertain model parameters demands for efficient uncertainty quantification, which can be done with the help of sensitivities or gradients [1,2]. However, the kinetic Monte Carlo particle tracing part for the neutrals (atoms and molecules) substantially complicates the calculation of accurate sensitivities. We show that Finite Differences (FD) give inappropriate sensitivities with up to a factor 10^4 relative statistical errors on the sensitivities. These enormous statistical errors originate from the unavoidable loss of correlation between the primal and perturbed particle trajectories. As an alternative, we present the use of Algorithmic Differentiation (AD) [3], which is automatically correlation-preserving and consequently gives up to a factor 10^5 statistical error reduction compared to the FD sensitivities for low-collisional conditions. However, there are issues with diverging sensitivities originating from a minority of long-lived particles in high-collisional conditions. We discuss similarities with sensitivity calculations for chaotic systems and we propose some solution strategies [4]. [1] Q. Wang., PhD thesis (2009) [2] S. Carli et al., Contrib. Plasma Phys. 62 (2021) [3] A. Griewank et al., proceedings of SIAM conference (2008) [4] Q. Wang, Journal of Comp. Phys. 235 (2013)

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MS9

Uncertainty Propagation in Multi-Scale Particle Transports

Coarse-grained modeling and simulation introduce considerable uncertainties between the field solutions of transport phenomena, and the real physics. To study the emergence, propagation and evolution of randomness from flight of particles to hydrodynamics poses great opportunities and challenges to develop both sound theories and reliable numerical algorithms. In this talk, we will discuss the similarities in principle and computing paradigm between kinetic theory and uncertainty quantification. A series physics-oriented stochastic kinetic schemes will be introduced. Asymptotic analysis and numerical experiments including neutral gases, quantum gases, and plasmas, will be presented to demonstrate the performance of the newly developed method.

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MS9

Stochastic Galerkin Particle Methods for Kinetic Equations of Plasmas with Uncertain Data

In this talk, we focus on a class of numerical methods that guarantees the preservation of main physical properties of kinetic models with uncertainties. In contrast to the direct application of classical uncertainty quantification methods, which may lead to the loss of structural properties, we discuss the construction of particle stochastic Galerkin schemes that are able to achieve high accuracy in the random space without losing nonnegativity of the solution and hyperbolicity of the macroscopic system. Applications of the developed methods are presented for kinetic equations of plasmas with uncertainties.

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MS10

Reduced Order Modeling for Bifurcation Analysis in Fluid-Structure Interaction Problems

This work consists in the development and analysis of an efficient reduced order model for the study of bifurcation phenomena governed by non-linear PDEs in fluid-structure interaction problems. We focused on a particular bifurcating phenomenon known as the Coanda effect, which concerns the Navier-Stokes equations' stationary solutions for an incompressible, newtonian and viscous fluid. We have chosen to address the particular case of a contraction-expansion channel because it represents a simplification aimed at analyzing a heart disease known as mitral valve regurgitation. The goal of our investigation was to generalize previous works conducted on such complex phenomenon, to understand how it is influenced by the introduction of an elastic structure at the interface of the fluid resolution domain. It should be noted that the reconstruction of the bifurcation diagrams related to a non-linear PDE requires considerable computational effort. That is why we have addressed the resolution by developing a reduced branch-wise algorithm based on a monolithic Proper Orthogonal Decomposition (POD) coupled with Galerkin Finite Elements. This approach optimizes the computational resources and provides results that can be applied in a multiple parameter context.

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MS10

Uncertainty Quantification and Data Assimilation: Engineering Applications Across Generalization and Specialization Thrusts

Multiphysics simulations are becoming essential sources of knowledge about complex engineering systems to inform design, maintenance and operational decisions. On one hand, uncertainty quantification and data assimilation methods offer incredible opportunities to improve the robustness of simulation-driven responses to generalize over larger domains; on the other hand, those are pivotal enablers of digital twins by allowing to specialize the virtual models in symbiosis with the real artifacts. These two competing dual thrusts shape a variety of computational frameworks. Specific methods and schemes will be discussed with examples across diagnostics and reliability assessment for sustainable development and aerospace applications. In addition, the open challenge of addressing those problems at scale is posed for a proactive conversation with the experts joining the forum.

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MS10

Stochastic Analysis of the Sensitivity of Atherosclerotic Plaque Onset in Carotides to Vessel Geometry

Atherosclerosis is an inflammatory cardiovascular disease that leads to a gradual narrowing of blood vessels due to the formation of plaques inside the artery. Over the years, the plaques can obstruct the blood flow to downstream vessels and organs. We aim to predict through CFD simulations the possible onset of carotid plaques and to analyze the influence of hemodynamic and geometric parameters on the early stages of the disease. We combine CFD simulations with a plaque growth model, in which ordinary differential equations describe the plaque growth linked to the wall shear stress and to Low-Density Lipoprotein concentration in the intima. The thickening of the vessel wall towards the arterial lumen is considered through a morphing procedure. We found in our previous studies that this model accurately predicts the onset region of the disease, and reasonably estimates the plaque growth rate in the early stages of the pathology. We consider herein a clinical dataset including the 3D segmented geometries of left and right carotids and the flow rate waveforms. From

the patient-specific case, we build a parametric geometry to single out which among the different geometrical parameters describing the carotid bifurcation is responsible for the possible onset and growth of the arteriosclerotic plaque. Continuous response surfaces in the parameter space are obtained by using stochastic sensitivity analysis techniques, as, e.g., the stochastic collocation method with sparse grids.

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MS10

Uq and Robust Optimization of Lifting Surfaces Made of Composite Laminates

Aeroelastic phenomena still represent a major challenge for modern aeronautical structures, which are designed to be light and slender, and, as such, proner to undergo aeroelastic instabilities. These phenomena are produced by complex non-linear interactions between aerodynamic forces and structural deformation, and they are strongly dependent on uncertainties (P. Beran et al, UQ in Aeroelasticity, Ann Rev of Fluid Mech, 2017). The use of composite laminates in aeronautical construction is a source of aleatory parameters (mainly, layer thicknesses and orientations), which have a strong impact on the structural aeroelastic response. In our work, we perform deterministic aeroelastic optimisation of aeronautical lifting surfaces made of composites laminates, and then uncertainty quantification of the aeroelastic response of the deterministic optima, thus showing their bimodal response and the need for a robust approach to aeroelastic optimisation. Several challenges have to be faced: on one hand, the computational burden of the aeroelastic analysis, which requires a proper choice of structural and aerodynamic models (in our work, we couple FEM and DLM models), as well as the use of metamodels; on the other hand, the curse of dimensionality due to the very high number of uncertain parameters in composite structures, which can be surpassed thanks to the polar parametrisation of anisotropic elastic properties (the use of polar elastic invariants is an original feature of our work).

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MS11

L^2 Regularization of Bilevel Problems on Probability Spaces

We consider a bilevel optimization problem constrained by the Kantorovich problem of optimal transport. We apply a quadratic L^2 regularization to the Kantorovich problem and study its effect on the bilevel problem. Using a reverse approximation argument, we present a result stating that the solution of the nonregularized bilevel problem can be approximated by sequences of solutions of the regularized bilevel problems. Finally, we present two application-oriented examples, the first of which is an inverse problem based on measurements of the transportation process, and the second of which is an optimal control problem in Wasserstein spaces.

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MS11

Bayesian Parameter Identification in Cahn-Hilliard Models for Biological Growth

We consider the inverse problem of estimating parameters in a model for tumor growth. The tumor is described by a phase field, that is the solution to a forth-order Cahn–Hilliard system with an additional equation that models diffusion of some nutrient. In total the model contains three phenomenological parameters: the tumor proliferation rate, the nutrient consumption rate, and the chemotactic sensitivity. We study the inverse problem within the Bayesian framework and construct the likelihood and noise for two typical observation settings. In one setting we observe the full tumor at some finite time while in the second setting we consider the volume of the tumor at a sequence of time points, thus finite dimensional data. We show the well-posedness of the posterior measure for both settings, building upon and improving the analytical results for this tumor model in [C. Kahle and K.F. Lam, Appl. Math. Optim. 82, (2020)]. A numerical example involving synthetic data is presented in which the posterior measure is numerically approximated by the Sequential Monte Carlo approach with tempering. This work is published in [C. Kahle, K.F. Lam, J. Latz, and E. Ullmann, SIAM/ASA JUQ 7(2) (2019)]

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MS11

Emulation for Multiphysics Simulations

To determine statistical information about a quantity of interest, one must potentially exercise the physical simulator that outputs this quantity for a large and varied set of input design points. These simulations can be extremely costly to perform which is a major limiting factor for understanding uncertainty under different operating conditions. This expense is even greater when the simulator models two or more types of coupled physics. If instead, one can develop a reliable reduced order model from running the simulator over a limited set of input design points, then the hope is one can evaluate the physics at additional input values without requiring simulation runs. In this work we consider Gaussian stochastic process (or GaSP) emulators which produce point estimates as well as uncertainty. Moreover, traditional GaSP emulators assume scalar quantities of interest. However most complex physical models output quantities that are functions of either space and time or both. We have developed emulators for coupled multiphysics models with vector output. Our primary application of interest is hydraulic fracture modeling in which injection and flow of fluids is coupled to fracture mechanics. Emulation can help us deduce whether typical metrics for assessing the effectiveness of such hydraulic stimulation results in creation of additional pore volume which is too expensive to assess via full physical simulation of different production scenarios.

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MS11

Tensor-Based OED for Bayesian Inverse Problems

Optimal Experimental Design (OED) involves designing optimal strategies for data acquisition, to minimize the uncertainty associated with reconstructions in Bayesian inverse problems. In some applications such as time-dependent problems, each design variable (e.g., sensors) can correspond to multiple data values (e.g., different time instances). We propose to address this using a tensor-based approach and derive efficient algorithms based on column subset selection. We will illustrate these algorithms on model problems involving time-dependent PDEs.

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MS12

Boundary-Constrained Gaussian Processes for Physical Modeling and Probabilistic Numerical Methods

Probabilistic numerics is an active field of research that seeks to construct stochastic analogues of numerical methods, including the solution of ordinary and partial differential equations. Probabilistic solvers for partial differential equations require the specification of flexible prior models that respect physical constraints while allowing for computational efficiencies of the sequential updates. We focus on state-space based probabilistic PDE solvers and describe advances in nonparametric modeling of system states with boundary constraints.

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MS12

Active Learning for Simulator Calibration

When acquisition of additional field data is cost prohibitive, reducing the prediction error of a statistical model is challenging. An alternative is to leverage simulator responses for improving field prediction via the Kennedy and O'Hagan (KOH) calibration framework. KOH models field data as the the output of a calibrated computer simulator plus a bias function, and often independent Gaussian Processes (GPs) are used for each when a simulator is computationally expensive. The closed form predictive variance and mean available from GPs allow for fast optimization of active learning criteria, reducing the computational burden of probing an expensive simulator. One criterion; integrated mean squared prediction error (IMSPE), aims to reduce the average predictive variance across the input space. Literature on active learning for acquiring simulator data for the purpose of improving field predictions within the KOH framework is sparse. First, we propose a closed form IMSPE criterion for use with KOH, termed KOH-IMSPE. We show the behavior of KOH-IMSPE, which interestingly acquires simulator data near calibration parameter estimates. Then we provide empirical Monte-Carlo results from toy examples. Last, we overview results from the motivating example: predicting equilibrium conditions of rare earth elements for a liquid-liquid extraction chemical process, as well as the particulars of where KOH-IMSPE is more advantageous than other design methodologies.

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MS12

Identifying Discontinuities Using Deep Gp Emulation

Sharp changes in the Quantity of Interest (QoI) within dynamical systems often indicate bifurcations or critical transitions within the investigated system. These instances can be found in switch-like behaviour in genomics and bifurcations in fluid dynamics. Identifying these sharp changes holds significance as they can result in significant changes within the system's inherent structures and behaviors. The challenges in the identification can be attributed to 1. In many situations, QoIs are estimated using computationally

expensive computer models, and only a limited number of evaluations are available. 2. The sharp change is a local measure which requires a high density of samples in its neighbourhood. An efficient approach localises these changes with minimal number of evaluations will be desirable. In this work, we introduce a branch-and-bound framework to iteratively construct the refined partitions of the input domain and select the next branch for exploration with a novel criterion. We demonstrate the efficacy of the proposed framework on several synthetic examples and a real-world problem derived from an ordinary differential equation.

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MS13

A Stochastic Maximum Principle Approach for Reinforcement Learning with Pa Rameterized Environment

In this work, we introduce a stochastic maximum principle (SMP) approach for solving the reinforcement learning problem with the assumption that the unknowns in the environment can be parameterized based on physics knowledge. For the development of numerical algorithms, we apply an effective online parameter estimation method as our exploration technique to estimate the environment parameter during the training procedure, and the exploitation for the optimal policy is achieved by an efficient backward action learning method for policy improvement under the SMP framework. Numerical experiments are presented to demonstrate that the SMP approach for reinforcement learning can produce reliable control policy, and the gradient descent type optimization in the SMP solver requires less training episodes compared with the standard dynamic programming principle based methods.

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MS13

A Novel Conditional Wasserstein GAN for Bayesian Inference

We present a new mathematically consistent formulation of conditional Wasserstein generative adversarial networks (cWGANs) for learning and sampling from conditional distributions in Bayesian inference problems. It modifies earlier variants of the architecture proposed by Adler et al. (2018) and Ray et al. (2022) in two fundamental ways: i) the gradient penalty term in the GAN loss makes use of gradients with respect to all input variables of the critic, and ii) once trained, samples are generated from the posterior by considering an open ball around the measurement. These two modifications are motivated by a convergence proof that ensures the learned conditional distribution weakly approximates the true conditional distribution governing the data. Through simple examples we also show that this leads to a more robust training process. Finally, we demonstrate that this approach can be used to solve complex inverse problems arising in mechanics.

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MS14

Uncertainty in Analytical Chemistry Measurements: Challenges and Implications

Destructive analytical chemistry of nuclear materials is used to support decision making in safeguards, nuclear forensics, and nuclear fuels fabrication. To provide defensible support to decision makers, the quality of data obtained by these analytical techniques must first be validated. At first glance, the task of estimating the accuracy and precision of analytical measurement processes looks like a simple application of textbook methods, but there are surprising practical challenges and the implications of uncertainty quantification are far-reaching. This talk will highlight statistical collaborations in analytical chemistry at LANL and our continuing work to provide meaningful estimates of uncertainty in measurement processes to support the decision making priorities of our collaborators.

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MS14

Image Deblurring and Uncertainty Propagation in Quantitative X-Ray Radiography

Quantitative X-ray radiography uses X-ray images to infer quantitative information about a captured scene. Inevitably, imperfections in the imaging process result in a blurry radiograph so deblurring is required to enhance the image. The blurring operation may be modeled as the convolution of the latent image with a point spread function. The point spread function characterizes the blur and is required to deblur the radiograph. However, the point spread function is not known in practice and must be estimated. Estimating the unknown point spread function introduces uncertainties that must be accounted for and quantified when assessing the deblurred image. In this talk, we will review a mathematical model for deblurring X-ray radiographs and explore how uncertainties propagate into measurements taken from the deblurred radiograph.

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MS14

Minimizing Uncertainty of Neutron Detection Systems in Mcnp Through Bayesian Machine Learning

Analyzing the path of neutrons through a system is a critical task performed throughout multiple scientific disciplines. Neutrons drive nuclear chain reactions, cause radiation damage to spacecraft, and facilitate a wide range of energy processes. Scientists commonly use computer codes to simulate the forward model of neutron transport. However, many practitioners are faced with the inverse problem: that is, given a target objective (e.g. optimize neutron detector efficiency) the goal is to find the parameters of the computer code that maximize this objective subject to some constraints (e.g. cost). We present a novel Bayesian optimization method capable of optimizing

neutron transport computer code and providing accurate uncertainty quantification. We apply our method to the problem of optimizing neutron detector efficiency while accurately quantifying the uncertainty in the efficiency.

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MS15

Seeing Perturbed Law-based Robustness Analysis of Epistemic Uncertainties in an Info-gap Framework

Uncertainty quantification in computer models has gained much consideration over the past decades. Many techniques are available to propagate aleatory uncertainty enabling the evaluation of risk-oriented quantities of interest such as low failure probabilities or high-order quantiles. However, these evaluations generally incorporate assumptions such as the choice of the input joint probability distribution which, in practice, may be subjective due to limited information. Robustness analysis is one way of addressing such assumptions by quantifying how their perturbations may impact the quantity of interest on which an industrial decision relies. This work takes a closer look at the info-gap robustness framework which assesses the degree of immunity of a decision to uncertainty affecting underlying assumptions. In particular, it is shown how this generic framework may be adapted to the robustness analysis of risk-oriented quantities of interest based on probabilistic representations. Moreover, close links between the info-gap framework and other metrics such as the Perturbed Law-based sensitivity Indices (PLI) are discussed. The comparison focuses on the different, yet complementary manners to perturb the input probabilistic assumptions and on the different interpretations offered by these robustness metrics.

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MS15

Robustness Analysis of Model Uncertainties Using Fisher Distance: the Case of Truncated Distributions

In many industrial applications, a computer code denoted G is used to simulate the physical behavior of a system or component. The output $Y = G(X_1, \ldots, X_d)$, sometimes referred as the system response quantity (SRQ), is a performance indicator or a parameter of the process submitted to operational or regulatory requirements. In a probabilistic UQ context, the probability distribution of Y represents the uncertainty induced by the uncertain input variables X_k of the problem, which can be affected by various uncertainty sources. These input uncertainties are usually modeled by parametric laws among a parametric family P_theta_theta ∈ Theta. The perturbed law robustness analysis framework (PL-RA) studies the impact of a perturbation of an input distribution on an output quantity of interest (QoI), which can typically be the alpha-quantile or super-quantile of Y for a given order α. The Fisher Information defines a metric in the parametric space where theta lies, giving it a Riemannian manifold structure. The derived Fisher-Rao geodesic distance can be used to measure the perturbation applied to input distributions. In most practical situations, bounds can be determined for the uncertain inputs, which modifies the Fisher geometry of the parametric space compared to the unbounded case. In this presentation, we will expose the general PL-RA framework and illustrate the geometry associated to input random variables with truncated supports.

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MS15

Differential Sensitivity in Discontinuous Models

Differential sensitivity measures provide valuable tools for interpreting complex computational models used in applications ranging from simulation to algorithmic prediction. Taking the derivative of the model output in direction of a model parameter can reveal input-output relations and the relative importance of model parameters and input variables. Nonetheless, it is unclear how such derivatives should be taken when the model function has discontinuities and/or input variables are discrete. We present a general framework for addressing such problems, considering derivatives of quantile-based output risk measures, with respect to distortions to random input variables (risk factors), which impact the model output through step-functions. We prove that, subject to weak technical conditions, the derivatives are well-defined and derive the corresponding formulas. We apply our results to the sensitivity analysis of compound risk models and to a numerical study of reinsurance credit risk in a multi-line insurance portfolio.

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MS15

Probabilistic Sensitivity Analysis for Engineering Design

Probability of failure is a commonly used metric to evaluate

a design in the presence of uncertainties. In order to quantify the impact of the input uncertainties, it is then desirable to conduct a sensitivity analysis where a change of the design metric is quantified subject to a change in the data or the design parameters. However, the failure probability depends on a specific design requirement, which itself can evolve during the design process. We present a new sensitivity metric using the Fisher Information Matrix (FIM) with respect to the input distribution parameters. As the FIM makes use of the entire distribution of the quantities of interest, it provides sensitivity information that is independent of the evolving design requirements. We will show that not only the FIM is closely linked to Entropy that is commonly used to quantify design complexity, the trace of the FIM also provides an upper bound of the sensitivity of failure probabilities.

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MS16

Bridging Classical Data Assimilation and Optimal Transport

Because optimal transport acts as displacement interpolation in physical space rather than as interpolation in value space, it can potentially avoid double penalty errors. As such it provides a very attractive metric for non-negative physical fields comparison, the Wasserstein distance, which could further be used in data assimilation for the geosciences. However, its theoretical formulation and implementation within typical data assimilation problems face conceptual challenges. We formulate the problem in a way that offers a unified view on both classical data assimilation and optimal transport. The resulting OTDA framework accounts for both the classical source of prior errors, background and observation, together with a Wasserstein barycentre in between the corresponding states. We show that the OTDA analysis can be decomposed as a simpler OTDA problem involving a single Wasserstein distance, followed by a Wasserstein barycentre problem which ignores the prior errors and can be seen as a McCann interpolant. We also propose a less enlightening but straightforward solution to the full OTDA problem, which includes the derivation of its analysis error covariance matrix. Thanks to these theoretical developments, we are able to extend the classical 3D-Var paradigm at the core of most classical data assimilation schemes. I will illustrate this talk with simple one– and two–dimensional examples that show the richness of the new types of analysis offered by this unification.

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MS16

Using Machine Learning, Data Assimilation and Their Combination to Improve a New Generation of Arctic Sea-Ice Models

We present an overview of the research efforts and results obtained in the context of the international project SASIP aimed at understanding and prediction the Arctic changes. We have been working on developing novel data assimilation, machine learning and their combination adapted to a new generation of sea-ice models that treats the ice as a brittle solid instead of as a fluid. These models present unique physical challenges such as sharp gradients, anisotropy and multifractality. We will first present an ensemble variational method to estimate the state and parameters of the sea-ice model based on synthetic, satellite-like, data. Second, we will show how to adapt the DA procedure to discontinuous Galerkin modeld, a modification that makes possible to assimilate very dense data and to develop a scale-aware localisation procedure. To incorporate multifractal, anisotropic, and stochastic-like processes in sea ice, we envision the combination of geophysical sea-ice models together with neural networks in a hybrid modelling setup. On the one hand, deep learning can surrogate computationally expensive sea-ice models, on the other hand, deep learning can parametrize subgrid-scale processes in sea-ice models and correct persisting model errors. Finally, we will show how to use neural networks to learn parametrization of the sea-ice melt ponds that have a major role on the albedo and thus on the general energy balance.

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MS16

Variational Optimal Transport Methods in Nonlinear Filtering

In this talk, I present a variational optimal-transportation (OT) method for nonlinear filtering, that aims at approximating the Brenier Optimal transport map from the prior to the posterior distribution, as a solution to a stochastic optimization problem. I discuss the relation of this approach to the feedback particle filter algorithm, and provide preliminary error analysis and numerical results that illustrates the performance of the algorithm in comparison with the sequential importance sampling particle filters.

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MS16

Learning Complex Turbulent Systems from Partial Observations with Stochastic Parameterizations

Discovering the underlying dynamics of complex systems from partial observational data is an important practical topic. This talk presents an iterative learning algorithm that alternates between identifying model structures, recovering unobserved variables, and estimating parameters. First, a causality-based learning approach is utilized for the sparse identification of model structures, which considers certain physics knowledge pre-learned from data. Next, a systematic nonlinear stochastic parameterization is built to characterize the time evolution of the unobserved variables. A closed analytic formula via efficient nonlinear data assimilation is exploited to sample the trajectories of the unobserved variables that advance a rapid parameter estimation. Numerical experiments show that the algorithm identifies the model structure and provides suitable stochastic parameterizations for systems with chaotic dynamics, multiscale structures, intermittency, and extreme events.

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MS17

Quasi Continuous Level Monte Carlo Methods for Nonlinear Stochastic Problems

The accurate and efficient estimation of moments of (functionals of) solutions to stochastic problems is of high interest in the field of uncertainty quantification. Adding nonlinearities to the underlying stochastic model may lead to large local effects in the solutions and inefficiencies in the moment estimation. Standard multilevel Monte Carlo methods (MLMC) are robust, but not able to efficiently account for these local effects, resulting in high computational cost. The standard continuous level Monte Carlo method (CLMC) can account for local solution features, but with its level distribution sampled by (pseudo) random numbers, it has a high variance. Thus, we consider the quasi continuous level Monte Carlo method (QCLMC), which combines adaptivity to local solution features via samplewise a-posteriori error estimates with quasi random numbers to sample its underlying continuous level distribution. Therefore, QCLMC has the potential of a high cost reduction and improved performance in comparison to MLMC and standard CLMC, which is demonstrated via an application to a random inviscid Burgers equation.

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MS17

Hybrid Methods for Nonlinear SPDE Models of Particle Systems

Interacting particle systems provide flexible and powerful models that are useful in many application areas such as sociology (agents), molecular dynamics (proteins) etc. However, particle systems with large numbers of particles are very complex and difficult to handle, both analytically and computationally. Therefore, a common strategy is to derive effective equations that describe the time evolution of the empirical particle density. An example of such equations is the well-studied singular Dean-Kawasaki equation. We will introduce nonlinear and non-Gaussian models that provide approximation of the evolution of the empirical density of a given particle system. We want to study numerical approximation of those type of non-linear SPDEs. In particular, since the unknown is the empirical density, the main goal is to provide numerical methods that preserve positivity. For that purpose we are considering the so called hybrid methods. The basic idea of the hybrid algorithm is to apply particle based method in the regions of the domain where the number density approximation becomes very small or in the regions where higher fidelity particle representation is required. Furthermore, we will discuss the application of these types of equations in the opinion dynamics. This is a joint work with J. Bell and Ann Almgren.

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MS17

Learing to Integrate

The parametrization of a random field by a countable or finite number of i.i.d. scalar random variables with a given simple distribution is essential for the numerical solution of differential equations with random distributed inputs, a key mathematical model in the propagation and quantification of uncertainty in technical or scientific computer simulations. The classical template of such representations is the Karhunen-Love expansion, which provides a linear modal expansion of a second-order random field in weighted eigenfunctions of its covariance operator with with uncorrelated scalar random coefficients. For Gaussian random fields, these random coefficients are also independent and themselves Gaussian. For random fields with more complex probability laws, such as generalized or Lvy fields such representations are more challenging to construct. In this work, we construct a parametric representation of a random field using an invertible neural net-

work (INN) and combine this with a sparse grid collocation method in order to sample realizations of a quantity of interest associated with the solution of a stationary diffusion equation.

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MS17

Analytic and Gevrey Class Regularity for Parametric Nonlinear Problems

We investigate a class of parametric elliptic nonlinear problems where the input data, such as diffusion coefficient and forcing term, may smoothly depend on the high-dimension parameter. The efficiency of various numerical approximations across the entire parameter space (generalized polynomial chaos, Quasi-Monte Carlo, etc) is closely related to the regularity of the solution with respect to the parameter, and hence the study of the precise estimation of the (mixed) derivatives of the solution is crucial. To that purpose, we propose the input data is analytic (or of Gevrey class) regularity and show that the same type of parametric regularity is valid for the solution. The key ingredient of the regularity proof is the combination of the alternative-to-factorial technique from our previous works, [Chernov and Le, 2023]. In particular, our findings regarding regularity have immediate implications for the convergence of Gaussian and Quasi-Monte Carlo quadrature designed for elliptic eigenvalue problems and semilinear reaction-diffusion problem.

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MS18

Conditional Optimal Transport: Amortized Inference for Bayesian Inverse Problems

We present a systematic study of conditional triangular transport maps in function spaces from the perspective of optimal transportation and with a view towards amortized Bayesian inference. More specifically, we develop a theory of constrained optimal transport problems that describe block-triangular Monge maps that characterize conditional measures along with their Kantorovich relaxations. This generalizes the theory of optimal triangular transport to infinite-dimensional Hilbert spaces with general cost functions. We further tailor our results to the case of Bayesian inference problems and obtain regularity estimates on the conditioning maps from the prior to the posterior. Finally, we present numerical experiments that demonstrate the computational applicability of our theoretical results for amortized and likelihood-free Bayesian inverse problems.

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MS18

Optimality of Pulse Energy for Photoacoustic Tomography

Photoacoustic tomography (PAT) is a rapidly evolving imaging technique that combines the high contrast of optical imaging with the high resolution of ultrasound imaging. When dealing with typically noisy measurement data, one aims to identify certain parameters in the governing PDEs for the photoacoustic tomography system. Therefore, an essential factor in estimating these parameters is the system's design, which typically involves multiple factors that can affect the accuracy of reconstruction. In this work, we employ a Bayesian approach to solving a PAT inverse problem with the goal of optimizing the laser pulse of the PAT system to minimize the uncertainty in the reconstructed parameters. Additionally, we account for wave propagation attenuation in the inverse problem of PAT, which is governed by a fractionally damped wave equation. Finally, we illustrate the effectiveness of our proposed method using a numerical simulation.

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MS18

Gaussian Process Surrogate for Bayesian Parameter Estimation Involving Incompressible Fluids

Gaussian processes are often used to model physical processes. In this project we seek to model physical processes involving the flow of incompressible fluids by using Gaussian processes that respect the incompressibility. The ultimate aim is to employ the Gaussian process as a surrogate for the forward map in Bayesian inverse problems involving incompressible fluids.

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MS19

Emulating sea-level rise across the world with uncertainty quantification

We present a comparative study of various emulation strategies for mapping between the Antarctic ice-sheet state and the consequent sea-level rise signal at locations across the globe. Emulators compared include a feed-

forward neural network, a conditional variational autoencoder, a random forest acting on a reduced-dimension space, and a Gaussian process acting on a reduced-dimension space. We find that the neural networks and Gaussian process based methods result in similar levels of predictive accuracy. However, post-hoc calibration of neural network predictions via simple regression methods provides better uncertainty quantification in terms of interval coverage than intervals derived from the Gaussian process emulator, for this particular scenario. We suggest that a future avenue of research is to extend the post-hoc calibration regression procedure by incorporating spatial information such as residual structure that is correlated spatially.

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MS19

When Are Approximate Bayesian Inference Methods Useful for Neural Networks? A Case Study in Chemical Composition Prediction from Spectral Measurements

Bayesian neural networks (BNNs) combine the remarkable flexibility of deep learning models with principled uncertainty quantification. However, poor scalability of traditional Bayesian inference methods such as MCMC has limited the utility of BNNs for uncertainty quantification (UQ). In this talk, we focus on recent advances in approximate Bayesian inference for BNNs and seek to evaluate, in the context of a real application, how useful these approximate inference methods are in providing UQ for scientific applications. As an example application, we consider prediction of chemical composition from laser-induced breakdown spectroscopy measured by the ChemCam instrument on the Mars rover Curiosity, which was designed to characterize Martian geology. We develop specialized BNNs for this task and apply multiple existing approximate inference methods, including variational inference and the linearized Laplace approximation, which can be viewed equivalently as a Gaussian process. We evaluate the quality of the posterior predictive distribution under different inference algorithms and touch on the utility of approximate inference schemes for other tasks, including model selection.

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MS19

Neural operator surrogates for ice-sheet models to accelerate probabilistic projections of sea-level rise

One of the most challenging and consequential problems in climate modeling is to provide probabilistic projections of sea-level rise, considering the uncertainty in ice-sheet dynamics. However, accurate quantification of the uncertainty requires running the ice-sheet models for a large number of parameter samples, which is often infeasible due to the cost of ice-sheet computational models. To address this issue, we propose a hybrid approach to approximate existing finite-element ice-sheet models at a fraction of their cost. In this approach, the finite-element model for the momentum equations, which is the most expensive part of an ice-sheet model, is replaced by a Deep Operator Network, while the classic finite-element discretization for the evolution of the ice thickness is retained. We show that the resulting hybrid model is accurate and an order of magnitude faster than the traditional finite-element model. The hybrid model can provide statistics of the glacier mass loss that are in agreement with those computed using the reference finite-element model. For increased accuracy, the hybrid model can be effectively used in a multi-fidelity strategy where a relatively small number of evaluations of the finite-element model (considered the high-fidelity model) are used together with evaluations of the hybrid model to improve the projection of the glacier mass loss.

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MS19

Regression Recalibration by Continuous Ranked Probability Score Minimization

In an era dominated by large-scale machine learning models, poor calibration severely limits the trustworthiness of the results. As we increasingly rely on complex systems, the task of recalibration becomes essential, where the objective is to find a mapping that adjusts the models original probabilistic prediction to a new, more reliable one. We explore a broad class of recalibration functions based on learning the optimal step function over a proper scoring rule. Using the continuous ranked probability score (CRPS) and applying predicted-mean binning, our approach outperforms the widely-used quantile recalibration method in terms of both calibration and sharpness, while maintaining its simplicity. We apply our method to a case study on the Pinatubo eruption climate dataset using a convolutional neural network model with dropout

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MS20

Inferring Ocean Transport Statistics with Probabilistic Neural Networks

Ocean currents transport heat, CO2, plankton, pollutants and more around the globe. While this transport is, in general, difficult to observe, valuable trajectory data is obtained from deployments of satellite-tracked drifting buoys known as drifters. Drifter data has been used to provide useful characterisations of ocean transport. However, the distribution of drifter trajectories is notoriously nonuniform and, in many regions, data is sparse. Using a probabilistic neural network trained to maximise the likelihood of observations from the Global Drifter Program, we model the single particle transition probability density function (pdf) of ocean surface drifters. This provides a comprehensive description of drifter dynamics allowing for the simulation of drifter trajectories as a Markov process and the estimation of a wealth of dynamical statistics without the need to revisit the raw data. An advantage of the neural network model is that it provides a continuous-in-space representation and avoids the need to discretize space, overcoming the challenges of dealing with nonuniform data. We also discuss the application of Bayesian neural networks to quantify uncertainty in the estimated statistics.

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MS20

An Adaptive Sampling Strategy for Multifidelity Uncertainty Quantification

Many problems in computational science, and uncertainty quantification (UQ) require the approximation of a high-dimensional function from noisy data. In many applications, data is costly to generate: for example, each sample may require a PDE solve. Therefore, it is imperative to develop highly sample-efficient models. Many methods are based on the fidelity data, high-fidelity models output data with high accuracy but it is expensive to compute. On the other hand, low-fidelity models output less accurate data but it is cheap to generate. Multi-fidelity models, which combine a high-fidelity model with several low-fidelity models, have shown accurate predictions using machine learning techniques. However, these proposed methods work with Monte Carlo sampling (MCS) or variations of MCS. Recently, Christoffel Sampling for Machine Learning (CS4ML) has shown accurate results approximating functions on arbitrary types of data. This is a general framework for active learning based on Christoffel functions. In this work, we propose an adaptive sampling strategy for Multi-fidelity UQ models. In particular, it integrates the multi-fidelity models and the sampling framework CS4ML to increase the sample efficiency of the model. Our novel approach is based on the Christoffel function on each latent space of the low-fidelity models to construct low-cost sample measures that will improve the approximation of the multi-fidelity model. We compare our method with respect to standard MCS.

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MS20

Stability for the Optimal Experimental Design in Bayesian Inverse Problems

The approximation problem in Bayesian inverse problems (BIPs) has been studied intensively in the last decade. In this work, we study some stability properties of the expected utility function for the optimal experimental design in BIPs. This is the "upstream' problem to inverse problems, which deals with how to design the experiments to acquire the data efficiently for the inference task. We provide a framework for this problem in a non-parametric setting and prove a convergence rate of the expected utility with respect to a likelihood perturbation. This rate is uniform over the design space and its sharpness in the general setting is demonstrated. To make the problem more concrete we proceed by considering non-linear Bayesian inverse problems with Gaussian likelihood and verify that the assumptions set out for the general case are satisfied and regain the stability of the expected utility with respect to perturbations to the observation map. Theoretical convergence rates are demonstrated numerically in different examples.

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MS20

Finite Time, Budget-Constrained Sequential Design of Experiments for Inverse Problems

Inverse problems frequently arise in engineering, physics, and other disciplines, where a system's properties are inferred from indirect data. Data collection for these problems often presents challenges: it can be time-consuming, expensive, or even dangerous, necessitating a systematic approach to decide which data to collect. Sequential uncertainty reduction (SUR) strategies address this by offering a Bayesian framework to design data collection plans that optimally decrease uncertainty about the target phenomenon. Although SUR has been successful in various applications, it often produces data collection plans that are impractical or challenging to implement. In this talk, we demonstrate how approximate dynamic programming can integrate experimental costs and global constraints into the SUR framework. This results in data collection plans that not only optimally reduce uncertainty but also align with defined budgets, enhancing the feasibility of sequential designs in real-world settings. This approach opens the door to more efficient and cost-effective solutions for inverse problems.

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MS21

Exploiting Structure via Nested Operator Inference in Physics-Based Learning

Highly accurate full-order models are often too expensive computationally to evaluate in predictive, real-time, or many-query applications. Projection-based model order reduction methods exploit the intrinsic low-dimensionality of the full-order solution manifold. These reduced-order models (ROMs) typically 1) achieve significant computational savings, 2) guarantee approximation accuracy through established error theory, and 3) remain interpretable through the governing equations. However, constructing ROMs via projection requires access to the full-order operators - a significant shortcoming for applications with legacy codes or commercial solvers. Operator Inference circumvents this requirement by learning the intrusive ROM from available full-order data and the structure of the governing equations. Under certain conditions, Operator Inference (OpInf) guarantees the exact reconstruction of the intrusive ROM, though meeting its data requirements in practice can be challenging for highly non-linear operators. In this talk, we introduce a nested extension to OpInf that exploits the projective structure of the reduced operators. While still guaranteeing exact reconstruction through a re-projection technique, nested OpInf significantly reduces the data requirement from polynomial scaling to O(1). The nested approach is thereby applicable for inferring ROMs with a high-order polynomial structure. We present results for the shallow-ice equations with 8th-order polynomials.

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MS21

Deep Learning Surrogate Models for Reservoir Modeling Applications

Assessing safety and environmental impacts of subsurface resource exploitation and management is critical and needs robust geomechanical models. However, uncertainties stemming from model assumptions, intrinsic variability of the parameters, and data errors challenge the prediction reliability. Sensitivity analysis and uncertainty quantification are essential to address this issue. In the absence of direct measurements, inverse modeling and stochastic data assimilation can offer a reliable solution, but in complex and large-scale settings the computational expense can become prohibitive. A proxy model based on Neural Networks (NNs) is developed to approximate the geomechanical results in a faulted reservoir application by leveraging laboratory tests and in-situ observations. The goal is to simulate fault slippage causing a potential induced seismicity. The NN-model is trained on snapshots generated by a full order model, hence it is valuable for real-time or multi-query applications, where fast computation is crucial. The edge of NNs is the capacity to approximate discontinuous functions, necessary to represent displacements in fault activation. Moreover, by constraining predictions to adhere to physical laws, the method can also ensure physical consistency. This work seeks to integrate deep learning with traditional modeling to reduce uncertainty in reservoir simulations, thereby enhancing prediction reliability and enabling robust simulations for design and optimization.

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MS21

Graph-Informed Neural Network and Discontinuity Learning

The multi-query nature of UQ analyses calls for the availability of surrogate models in case of rather complex underlying problems. In order to reduce the computational complexity of the process, recent literature shows that it is worth considering the application of neural networks (NN) to perform regression tasks. In several applications, network analyses come into play; in this framework, the authors have recently proposed a new type of NN layer designed for regression tasks on graphs, called graph-informed (GI) layer. Recently, we exploited GI-layers to develop a new algorithm based on sparse grids for detecting discontinuity points of n-dimensional piece-wise continuous functions; this task is of interest in UQ analyses, as in some applications the Quantity of Interest may be a discontinuous function in the space of stochastic parameters, thus preventing from the effective application of stochastic collocation strategies. The underlying graph structure is associated with the sparse grid in use; the algorithm leverages the graph structure to identify the discontinuity interface of piece-wise continuous functions, using suitable detectors of grid points close to the discontinuity interface. Nonetheless, deterministic detectors are expensive, especially in high-dimensional domains. Therefore, we also introduce NN-based detectors, trained on synthetic data. The NN-based detectors proved to have very good abilities, especially if Graph-Informed Neural Networks are used.

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MS22

On Anisotropic Adaptivity for Stochastic Hyperbolic Partial Differential Equations

Hyperbolic partial differential equations (PDEs) can exhibit the formation of discontinuities in finite time from smooth initial conditions. This poses significant difficulties to accurate and efficient numerical simulations of theoretical and physical phenomena modeled by such PDEs. When further augmented by explicit uncertainties, numerical methods require precise capture of solution behavior

to reproduce statistical moments and probability densities. To deliver the properties of accuracy and efficiency, given the intricate relationship between the physical and stochastic spaces, we consider in this talk an anisotropic adaptivity framework for stochastic hyperbolic PDEs under a parametric setting. To drive more effective computational resource allocations, we propose an a posteriori error estimator and smoothness indicator pair that automates the insertion of new degrees of freedom during the evolution of the target PDEs. Moreover, we exploit the properties of the physical and stochastic spaces to sculpt directional refinements that improve efficiency while preserving physical constraints, namely conservation. Finally, we demonstrate the enhanced convergence rates afforded by the proposed method in comparison to global refinements.

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MS22

Adaptive Arbitrary Multi-Resolution Polynomial Chaos-Based Bayesian Active Learning for PDE Calibration

Calibration of mathematical models, which are often described by PDEs, is one of the crucial tasks in mathematical modeling and engineering sciences. Inverse Bayesian parameter inference is a well-established class of methods to estimate distributions of the input parameters. Unfortunately, at least the straightforward application of Bayesian parameter inference requires a comparatively high number of model evaluations. To tackle this problem, we employ an adaptive version of arbitrary Multi-Resolution Polynomial Chaos (aMR-PC), which extends a well-established data-driven arbitrary Polynomial Chaos as a model surrogate for Bayesian parameter inference. More precisely, aMR-PC uses the multi-resolution/multi-element Ansatz to reduce the Gibbs phenomenon related oscillations that are typical for the application of the PCE-based surrogate models in context of non-linear convection dominated problems. However, in many real-world applications' high computational costs of each model evaluation require further reduction of the number of training samples. To face this challenge, we propose to employ Bayesian active learning strategies to obtain the training samples which are relevant to the model calibration. This talk focuses on the construction of adaptive aMR-PC-based surrogate models and present application of Bayesian inference on aMR-PC surrogate models trained on samples proposed by Bayesian active learning.

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MS22

A Hybrid AMR-Low-Rank-Algorithm for the Boltzmann Bgk-Equation

The Boltzmann equation describes the time evolution of a particle distribution function in a six-dimensional position-velocity phase space. The exponential growth in computational complexity often challenges a grid-based approach to modeling the Boltzmann equation as the dimensionality grows. Scalable low-rank tensor decomposition techniques have recently been developed with applications to high-dimension PDEs to address this issue. Despite the remarkable progress made in the community, low-rank structures in the phase-space are not evident in realistic engineering systems with complex geometries (e.g., electric propulsion systems and fusion reactors), where discontinuities, shocks, complex boundary conditions, and material-dependent physics (e.g., collisions, fusion reactions, ionization/excitation, charge-exchange processes) pose formidable challenges. In this talk, we propose a novel hybrid algorithm where quad-tree adaptive mesh refinement (AMR) is applied in real space while a low-rank approximation is applied in the velocity space. The AMR algorithm efficiently handles challenges pertaining to complex structures in real space, while the low-rank formulation targets dimensionality challenges in the velocity space. We present preliminary results on the new algorithm applied to challenging multi-dimensional gas kinetics problems.

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MS23

Machine Learning of Model Errors in Dynamical Systems

The development of data-informed predictive models for dynamical systems is of widespread interest in many disciplines. We present a unifying framework for blending mechanistic and machine-learning approaches to identify dynamical systems from noisily and partially observed data. We compare pure data-driven learning with hybrid models which incorporate imperfect domain knowledge. Our formulation is agnostic to the chosen machine learning model, is presented in both continuous and discrete-time settings, and is compatible both with model errors that exhibit substantial memory and errors that are memoryless. We will present formulations and experiments to examine

data-driven point-wise and distributional estimates of differential equations in these settings.

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MS23

Stochastic Model-Based Glycemic Management for Intensive Care Unit Patients

Uncertainty quantification (UQ) is essential in forecasting and prediction in medical settings. Healthcare providers want to know the uncertainty in the computational model-based predictions and forecasts for better-informed decisions. Because of critical illness and frequent interventions, intensive care unit patients' blood glucose (BG) levels show nonstationary behavior, which increases the importance of UQ for model-based forecasting and control. Moreover, the available sparse data, i.e., at most 10-15 BG measurements per day, make it harder to obtain accurate forecasts. We developed a physiology-based, linear, stochastic model representing BG dynamics to account for these limitations, obtain clinically useful BG forecasting, and eventually use it for BG control. The model output is a Gaussian stochastic process. The mean represents the mean BG behavior, and the variance quantifies the amplitude of BG oscillations. When the mean is accompanied by the 2-stdev bands, the model naturally provides UQ in the forecasts. The mathematical simplicity of the model allows us to use it with linear quadratic Gaussian control to estimate the optimal action (here, exogenous insulin to be delivered) to maintain BG levels in a predefined healthy range. Our results with virtual patients and real-world retrospective data show that the resulting model-based personalized controller provides appropriate insulin amounts to maintain healthy glycemic regulation.

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MS23

Leveraging Model-Inferred Distributional Information to Improve Phenotype Resolution

In physiological applications targeting real clinical contexts, estimated model parameters may have large errors and uncertainties that arise from numerous sources, limiting the quality of downstream analysis. Luckily, modern inversion methods and data assimilation (DA) can identify possibilities for parameter configurations or approximate their distribution. Such uncertainty information can be incorporated into subsequent synthesis and interpretation processes. We present recent applications using uncertainty-enriched features to identify phenotypes of glucose-insulin systems and lung-ventilator interactions through the analysis of clinical data. Variability and internal irregularities in these systems may indicate important patient/system features. Classifying features and their associated uncertainty improves phenotype resolution, and we discuss the potential practical benefits of this improvement on clinical utility.

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MS23

Data Assimilation Through Optimal Transport

A methodology is proposed for the analysis of medical data, including data assimilation and decision-making support, based on the optimal transport barycenter problem. In order to simulate a conditional distribution $\rho(x|z_*)$ from data pairs (x^i, z^i), one first removes from x the variability attributable to z through a map $y = T(x, z)$, and then restores this variability for the particular target value z_*: $y^i = T(x^i, z^i)$, $x^i_* = T^{-1}(y^i, z_*)$. If a model for the process is available, its parameters and latent variables can be identified through a second, parametric map $w = Q(x, a)$, through the minimization of the expected value of a cost function $c(Q(x, a), T(x, z))$. Additional latent variables can be discovered through the solution through flows in phase-space of a multi-agent game.

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MS24

A Sequential Discretisation Scheme for Stochastic (partial) Differential Equations and Its Application to Bayesian Filtering

Many real-world systems are modelled by continuous-time state-space models. In these models, the dynamics of the signal of interest (or state) are described by stochastic differential equations (SDEs) or stochastic partial differential equations (SPDEs) and observed data are noisy, partial and often through nonlinear mappings. In this setup, Bayesian filters aim at the computation of the conditional probability law of the state given the available observations. The practical implementation of Bayesian filters requires the discretisation of the SDE/SPDE (a process that entails an error with respect to the original model) and the choice of discretisation scheme has an impact on the performance of the filters. Here, we introduce a predictor-corrector discretisation scheme for the numerical integration of SDEs/SPDEs and prove that it converges with weak order 1.0. The new scheme builds up sequentially and recursively in the dimension of the state, hence making it suitable for high-dimensional models. We introduce a theoretical analysis of the error due to the new discretisation method (and other weak schemes) when used as a building block in discrete-time Bayesian filters for continuous-time systems. Finally, we discuss the performance of several filters that incorporate the proposed sequential scheme. The numerical experiments show that the filters employing the new scheme can operate with larger time steps, smaller Monte Carlo ensembles and noisier observations.

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MS24

Connections Between Sequential Filtering and Dynamical Systems in Evolutionary Biology

Sequential learning or state estimation is a fundamental goal of many tasks in science and engineering. Of particular importance is in quantifying the uncertainty in those state estimates in real time, particularly in applications where data arrives in real time and rapid estimates are required. It has long been posited that there is a connection between evolutionary dynamics and sequential learning methods. In this talk I discuss recent work that draws precise connections between nonlinear filtering and replicator dynamics, with special focus on the linear Gaussian setting and connections to various Kalman dynamics. It is hoped this work will spur further research into exchanges between sequential learning and evolutionary biology.

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MS24

Edge-preserving Priors Based on Gaussian Scale Mixtures for Bayesian Inverse Problems

In large-scale inverse problems like image deblurring and X-ray computed tomography, preserving sharp features in the solution is crucial. Within the Bayesian framework for inverse problems, this task can be achieved using Markov random field priors that follow heavy-tailed probability distributions. In this study, we introduce a family of edge-preserving priors that combines the structure of first-order Markov random fields with Student's t distribution. To enhance the efficiency of posterior sampling, we exploit the Gaussian scale mixture representation of this heavy-tailed distribution, employing a hierarchical Gibbs sampler. We demonstrate the performance of the prior on linear Bayesian inverse problems.

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MS24

Optimal Matrix-Weighted Poincar Inequality for Preconditioning Langevin Dynamics

The main challenges faced by sampling methods are the multi-modality and the heavy-tails of the target probability distributions. Traditional algorithms like Markov Chain Monte Carlo (MCMC) struggle to effectively explore the complete landscape of the target distribution, leading to poor numerical performance. We address this issue by leveraging recent advancements in Markovian semigroup theory, including the notion of Stein Kernel and Moment Map. Based on these, we propose a preconditioning strategy for Langevin stochastic differential equations which enables rapid jump across various modes and tails of the target measure. Our approach is based on a matrix-weighted variant of the Poincar inequality, for which we optimize the constant. We showcase the effectiveness of our approach through experiments on challenging test cases known to be difficult to sample from.

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MS25

Solving Bayesian Inverse Problems Via Approximation of Joint Flows

In this talk we will first discuss the robustness of conditional generative models. Based on this perspective we are interested in whether training a conditional generator to minimize the distance to the joint distribution gives any guarantees on the expected posterior distance. For KL, equality holds between these quantities by the chain rule. We establish similar bounds for the Energy distance and discuss the Wasserstein case. These results will be underlined by numerical experiments.

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MS25

Solving Stochastic Differential Equations Using Deep Operator Networks

Stochastic differential equations (SDEs) have emerged as a crucial framework for modelling systems affected by random factors, thereby introducing a stochastic element into solutions. They find extensive use in finance, optimal control, generative models and physical systems. Recently, polynomial chaos expansions have proved to be highly successful in the area of uncertainty quantification of parametric partial differential equations. To date, the potential of polynomial chaos expansion has not been fully exploited for SDE. The main disadvantage in the truncated polynomial chaos expansion is that the number of components grows drastically with the maximum degree of polynomial chaos and the number of basis elements. This talk introduces a new model class, SDEONet, which is founded on the Wiener chaos expansion structure and the concept of Deep Operator Networks. This model aims to tackle the issue of exponential complexity by learning a sparse truncation of the Wiener chaos expansion. Experiments have validated the suggested approach in 1D and higher dimensions, and we obtain encouraging results.

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MS25

Approximating Langevin Monte Carlo with Resnet-Like Neural Network Architectures

Langevin Monte Carlo (LMC) describes the procedure of (approximately) sampling from a given probability density by discretizing a corresponding Langevin dynamics with the Euler-Maruyama scheme. In this talk, we consider approximations of the LMC algorithm with Res-Net like Neural Network architectures and perform error analysis in the 2-Wasserstein distance. The proposed architecture imitates LMC by composing feed-forward Neural Networks, each of which approximates the drift term with epsilon accuracy in an appropriate L2-space defined by the current law of the process. We show that the network architecture can achieve arbitrary accuracy for smooth, log-concave probability densities and give complexity bounds.

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MS26

Gaussian Process Learning of Nonlinear Dynamical Systems

One of the pivotal tasks in scientific machine learning is to discover underlying dynamical systems from time series data. Many methods for such dynamics learning explicitly require the derivatives of state data, which are not directly available and can be approximated conventionally by finite differences. However, the discrete approximations of time derivatives may result in a poor estimation when state data are scarce and/or corrupted by noise, thus compromising the predictiveness of the learned dynamical models. To overcome this technical hurdle, we propose a new method that learns nonlinear dynamics through a Bayeisan inference of characterizing model parameters. This method leverages a Gaussian process representation of states, and constructs a likelihood function using the correlation between state data and their derivatives, yet prevents explicit evaluations of time derivatives. Through a Bayesian scheme, a probabilistic estimate of the model parameters is given by the posterior distribution, and thus a quantification is facilitated for uncertainties from noisy state data and the learning process. Specifically, we will discuss the applicability of the proposed method to two typical scenarios: 1) parameter inference with a known structure of the dynamical system, and 2) parametric approximation of the dynamical system without prior knowledge.

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MS26

Learning Solution Operators for PDEs with Uncertainty

We provide a Bayesian formulation of the problem of learning solution operators of PDEs in the formalism of Gaussian processes. We consider recent deep architectures (neural operators) that have shown promising results in tackling the task of learning PDE solution operators. The current state of the art for these models does not provide explicit uncertainty quantification. We first provide an analytic Bayesian treatment of the shallow version of neural operators by directly inferring the solution operator (Greens function). We then introduce the concept of function-valued Gaussian processes to extend this analytic treatment to Fourier neural operators using approximate methods from Bayesian deep learning. This results in an (approximate Gaussian) belief over operators between Banach spaces.

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MS26

Learning Spatio-Temporal Dynamics of Parametrized Systems with Neural Networks

The numerical approximation of many query problems, such as forward and inverse uncertainty quantification (UQ), requires numerous evaluations of the map between inputs and quantities of interest. When this map encodes complex spatiotemporal dynamics, its approximation requires high-dimensional computationally intensive numerical discretizations of differential models, creating bottlenecks in UQ routines. Reduced-order models (ROMs) based on dimensionality reduction techniques can limit this computational burden, but they do not always guarantee high computational efficiency in the case of elevated spatiotemporal variability. In this talk, we present a new class of surrogate models based on neural networks, called Latent Dynamics Networks (LDNets), which are capable of reconstructing low-dimensional intrinsic (i.e., over a latent space) dynamics of a non-Markovian dynamical system. The LDnet architecture allows meshless prediction of quantities of interest based on the query point and the dynamics in the latent space, without ever having to operate in the high-dimensional space during both training and prediction. LDnet allows neural network parameters to be shared among query points, reducing the training time and improving accuracy and generalization properties over state-of-the-art ROMs.

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MS26

Learning Functions, Operators and Dynamical Systems with Kernels

Supervised machine learning is concerned with the problem of estimating a function of interest from a random set of input/output pairs. While, classically, real valued functions are considered, there is a growing interest in estimating more complex maps such as linear and nonlinear operators. In this talk , I will describe how these questions can be tackled using kernel methods. I will show how many known results for scalar valued functions seamlessly extend to operators. Then, I will describe how this approach can be used to learn dynamical systems by estimating the corresponding Koopman operator.

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MS27

Generative Hyperplasticity with Physics-Informed Probabilistic Diffusion Fields

Data-driven methods for computational mechanics have become popular due to their ability to capture complex material behavior. We have contributed to the field by proposing machine learning architectures that a priori satisfy polyconvexity and positive energy dissipation of soft viscoelastic materials. Our framework is based on the monotonicity of neural ordinary differential equations (NODEs), which we use as building blocks to represent derivative functions of convex energy and dissipation potentials. However, data-driven constitutive modeling has focused on the response of individual material samples, ignoring the uncertainty across a material family. This is particularly problematic for materials with variation across a population such as soft tissues. To capture this uncertainty, here we show that the joint probability density of NODE parameters describing the mechanical behavior of samples from a population can be represented with probabilistic diffusion models. The method outperforms density estimation methods such as mixture of Gaussians. The trained probabilistic diffusion model can be used to generate new samples from the population and even samples conditioned on new observations. Lastly, we extend the Euler-Maruyama scheme of the original reverse stochastic differential equation to take sample fields from a Gaussian process and turn them into spatially correlated fields of material properties with controllable length scales.

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MS27

Deep-Learning Based Conditional Probability Estimation: Diffusion Or Adversarial?

Deep learning based conditional generative models offer a novel approach for solving large scale probabilistic inference problems. Of these, conditional Wasserstein generative adversarial networks (CWGANs) and conditional diffusion networks are two popular choices. In this talk we will explore the application of both these networks to chal-

lenging problems and compare their performance. We will also discuss how some of the drawbacks of these methods may be addressed.

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MS27

Efficient Neural Network Approaches for Conditional Optimal Transport with Applications in Bayesian Inference

Efficient simulation of *conditional* relationships between two sets of variables is a key computational challenge in Bayesian inference. Sample-driven approaches to this problem are particularly flexible and well-suited to the setting of simulation-based Bayesian inference—where the prior and/or likelihood are intractable. Transportation of measure offers a general framework for solving these problems, by representing the "target conditional distributions as transformations of a tractable reference distribution. Conditional optimal transport (COT) maps are a canonical choice within this framework, with desirable properties. Yet COT problems remain difficult to solve even in moderate dimensions. We present two neural network approaches for approximately solving COT problems and demonstrate their effectiveness using benchmark datasets and applications in Bayesian inverse problems. Our approaches exploit the structure of the static and dynamic formulations of the COT problem, respectively: PCP-Map models conditional transports as the gradient of a partially input convex neural network and uses an efficient numerical implementation to reduce training time compared to state-of-the-art alternatives. COT-Flow models conditional transports via the flow of a regularized neural ODE; it is slower to train, but offers faster sampling. Our experiments use a simple heuristic to select hyperparameters, enabling convenient model adaptations for new problems.

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MS28

Multilevel Monte Carlo Methods with Smoothing

We consider the computational efficiency of Monte Carlo (MC) and Multilevel Monte Carlo (MLMC) methods applied to elliptic partial differential equations with random coefficients. These models arise, for example, in groundwater flow modelling, where a common configuration for the unknown parameter is a random field. We make use of the circulant embedding procedure for sampling from the aforementioned coefficient. Then, to further improve the computational complexity of the MLMC estimator, we devise and implement the smoothing technique integrated into the circulant embedding method. This allows to choose the coarsest mesh on the first level of MLMC independently of the correlation length of the covariance function of the random field, leading to considerable savings in computational cost. We illustrate this with numerical experiments, where we consider different correlation lengths for the random parameter.

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MS28

Quantifying Uncertainties Beyond Moments via the Multilevel Monte Carlo Method

In recent years, the multilevel Monte Carlo (MLMC) method has been established as a computationally efficient sampling method for quantifying uncertainties in computational models. In particular, the method's non-intrusive nature enables the use of MLMC as a general-purpose method, such as for the forward propagation of model uncertainties by approximating expected values of random system outputs, resulting in many theoretical, methodological, and algorithmic developments in the last years. Some applications, however, require assessing a random system output's distribution beyond expected values, including risk-averse prediction, optimization, and decision-making processes under uncertainties. An estimation via the MLMC method of such statistics that cannot be expressed as an expected value is complex and requires special treatment. In this talk, we will describe methodologies for constructing MLMC estimators of central moments (e.g., variances), distribution functions, and robustness indicators, focusing on quantifying "tail" risks using quantiles (value-at-risk) or conditional values-at-risk. Furthermore, we will outline practical procedures for an efficient and robust adaptive algorithm.

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MS28

Practical Large-Scale UQ with tinyDA: Adaptivity, Surrogates and Error Models

The application of numerical Bayesian methods for Uncertainty Quantification has grown rapidly in the last two decades. However, this development has not fully permeated into the realm of large-scale inverse problems. The

main reason for this discrepancy is the complexity of exploring the (often high-dimensional) posterior distribution with little prior knowledge of its shape, making Markov Chain Monte Carlo (MCMC) inefficient and costly. There have been several sophisticated algorithmic developments to attempt to alleviate this problem, of which most rely on higher-order geometric properties of the posterior distribution. However, in practice, exploiting such properties is often not computationally tractable, and adaptive and approximate inference methods are preferable. Such methods include adaptive MCMC, surrogate MCMC, and approximation error modelling. In this talk, I will give a brief overview of the Multilevel Delayed Acceptance (MLDA) MCMC package tinyDA, which leverages both multilevel model hierarchies, adaptive proposals, and approximation error models to significantly reduce both the upfront human labour cost of setting up the MCMC and the computational burden of converging to the Bayesian posterior distribution. I will give a brief overview of surrogate MCMC as well as approximation error models for multilevel MCMC, and present examples of large-scale Bayesian inverse problems that were solved using these methods.

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MS28

Combining Noisy Well Data and Expert Knowledge in a Bayesian Calibration of a Flow Model under Uncertainties: An Application to Solute Transport in the Ticino Basin

In this talk we present the results of a case-study aimed at providing a UQ analysis of solute travel times in groundwater in the basin of the Ticino River (northern Italy), starting from well data collected over a month in summer 2014. We consider a steady-state groundwater flow model (developed in MODFLOW) and perform a sensitivity analysis using the Morris method to discard uninfluential parameters. We then employ Bayesian inversion (with Gaussian approximation) to obtain a data-informed posterior pdf for the remaining parameters, and propagate these pdfs to travel times computed by particle tracking (MODPATH). The likelihood function employed in the Bayesian inversion takes into account both well measurements and expert knowledge about the extent of the springs in the domain under study.

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MS29

Uncertainty Quantification in Atomistic Simulations Using Interatomic Potentials

I will discuss how UQ frameworks can be used to quantify and propagate the aleatoric and epistemic uncertanties associated with atomistic models of materials. Such simulations often rely on interatomic potentials to access greater time- and length- scales than those accessible to first principles methods such as density functional theory (DFT). However, since a parameterised potential typically cannot reproduce the true potential energy surface of a given system, we should expect a decrease in accuracy and increase in error in quantities of interest calculated from simulations. Quantifying the uncertainty on the outputs of atomistic simulations is thus an important, necessary step so that there is confidence in results and available metrics to explore improvements in said simulations. Here, we adress this reseach question by forming ensembles of Atomic Cluster Expansion (ACE) potentials, and using conformal prediction with DFT training data to provide meaningful, calibrated error bars on several quantities of interest for an example silicon model: the bulk moduluus, elastic constants, relaxed vacancy formation energy, and the vacancy migration barrier. Finally, we evaluate the effects on uncertainty bounds of using a range of different potentials and training sets.

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MS29

Indicator Configurations: An Information-Matching Method of Data Reduction for Training Interatomic Potential

Interatomic potentials (IPs) are often trained by fitting IP parameters to energies, atomic forces, or similar quantities for many atomic configurations. These training quantities are typically obtained from DFT calculations, and collecting data from enough unique configurations to constrain all IP parameters is computationally expensive. A critical problem is identifying when the training data is sufficient to constrain the predictions of the IP for material properties of interest. We present an information-matching method for selecting a minimal set of configurations, i.e., indicator configurations, that constrain the predictions of an IP for target material properties. Central to our analysis is the Fisher Information Matrix (FIM), that quantifies the information that the data carries about the IP parameters. We calculate the FIM for the target quantities of interest and for, e.g., the energy and forces of each candidate configuration. Then, we down-select from these candidate configurations so that their combined FIM matches that of the quantities of interest, i.e., the indicator configurations are those whose information content is the same as the target predictions. We demonstrate this method on the Stillinger-Weber potential for several systems and target materials properties. In addition to improving the

efficiency of the data-generation process, the indicator configurations reveal the physics and mechanisms relevant to the materials properties of interest.

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MS30

Uncertainty Quantification and Sensitivity Analysis in Conjugate Heat Transfer Simulations for Predicting Flashback Limits of Hydrogen-Enriched Flames

Hydrogen is increasingly considered a viable option for decarbonization across various sectors, offering an alternative to natural gas while maintaining existing combustion-based systems. However, its higher reactivity compared to natural gas poses a significant risk of flashback. In this study, a comprehensive sensitivity analysis on hydrogen-enriched flames in multi-slit burners is conducted, with a specific focus on how material properties and geometrical parameters influence flashback propensity. The approach integrates Computational Fluid Dynamics (CFD) simulations with the sparse-grid stochastic collocation method to efficiently perform this analysis. 2D transient numerical simulations are carried out, accounting for Conjugate Heat Transfer (CHT) between the fluid and the solid walls, to accurately predict the burner temperature and the flashback velocity. The stochastic sensitivity analysis is employed to assess the relative importance of the input parameters, utilizing sparse grid methods to minimize the number of resource-intensive simulations. Through this approach, comprehensive maps are generated, detailing flashback velocities and burner temperatures as burner material properties and geometry parameters vary. Ultimately, this methodology contributes to the development of innovative burners capable of safely handling various hydrogen-enriched mixtures, including up to 100% hydrogen.

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MS30

BayeSAF: A Bayesian Framework for Modeling Physicochemical Surrogates of Sustainable Alternative Fuels

The endorsement of climate neutrality policies strengthens the ambition to identify sustainable alternatives to fossil fuels for any category of transportation systems. In this context, the aviation industry envisages net-zero carbon targets to be achieved by mid-century. As evidenced by recent initiatives of international institutions, one solution to ensure a transition to a low-carbon future is blending conventional and drop-in sustainable aviation fuels. However, the unusual properties of alternative jet fuels may profoundly impact the performance and operability of engines. Thus, adequate characterization of non-standard fuel blends is crucial to applying computational fluid dynamics (CFD) to assess the performance of alternatively fueled combustion devices. Existing strategies to formulate surrogate mixtures that emulate the physicochemical properties of real fuels typically hinge on genetic optimization algorithms, which address complex combustion behaviors by replicating one-parameter combustion property targets (CPTs), e.g., the cetane number (CN). In the present work, we illustrate a novel Bayesian framework called BayeSAF, which fosters employing polynomial chaos expansion (PCE) representations of the major chemical observables under engine-relevant conditions, such as the ignition delay time, instead of lumped CPTs. This way, a Bayesian-based emulation of physicochemical properties paves the way toward using ad-hoc surrogate mixtures in CFD codes.

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MS30

Model-to-Model Bayesian Calibration of a Chemical Reactor Network for Pollutant Emission Predictions of An Ammonia-Fuelled Multistage Combustor

Low-fidelity, cost-effective, physics-based models are useful for assessing the environmental performance of novel combustion systems, especially those utilizing alternative fuels, like hydrogen and ammonia. However, these models require calibration and quantification of their limitations

to be reliable predictive tools. This talk presents a framework for calibrating a simplified Chemical Reactor Network model using higher-fidelity Computational Fluid Dynamics data from a micro-gas-turbine-like combustor fueled with pure ammonia. A Bayesian inference strategy that explicitly accounts for model error is used to calibrate the most relevant CRN parameters based on NO emissions data from CFD simulations and to estimate the model's structural uncertainty. The calibrated CRN model accurately predicts NO emissions within the design space and can extrapolate reasonably well to conditions outside the calibration range. By utilizing this framework, low-fidelity models can be employed to explore various operating conditions during the preliminary design of innovative combustion systems.

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MS30

CFD Uncertainty Quantification Based on Stochastic Spectral Methods

In the realm of modern technology, the demand for reliable and accurate simulation-based predictions of technical processes is of paramount importance. This is particularly true for safety-critical applications like hydrogen facility operations and reactor safety. Severe accidents in these fields involve buoyancy-induced mixing processes, with complex interactions between air and hydrogen. Such complexity, coupled with potential risks involved, highlights the necessity of developing robust and reliable predictive models. However, these models are inevitably afflicted by uncertainties which, if unaddressed, could have significant consequences. Our objective is to address these uncertainties in CFD model predictions on a technical scale. We focus on the stochastic modeling of time-dependent stochastic processes. To achieve this, we employ Polynomial Chaos Expansion in conjunction with Karhunen-Love Expansion. Additionally, we incorporate complementary techniques like Stochastic Model Composition, which realigns temporal non-linear effects, thereby improving the overall response approximation. The obtained UQ results include a thorough probabilistic representation of time-dependent response quantities including an error estimation and variance-based decomposition. The methodology demonstrates promising prospects for UQ of technical-scale computations, given its efficiency and precision in building stochastic models.

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MS31

Efficient Physics-informed Machine Learning Algorithms for Flow Problems

Modeling and simulation of compressible turbulent mixing induced by hydrodynamics instabilities have been a challenging problem due to the complex interface dynamics. The fine-scale structures within the mixing zone need to be resolved to capture the interface dynamics accurately. The physics-informed neural networks (PINNs) algorithm which takes into account the Euler/Navier Stokes partial differential equations is used to make predictions on the scale-dependent dynamics of these hydrodynamic instabilities. One of the challenges of the PINNs algorithm is to capture the shock and contact discontinues accurately and efficiently. The computation of the loss and gradient becomes very expensive due to the multiscale nature of flow problems. We investigate the effect of the residual-based adaptive refinement technique during the training process to improve the efficiency of the PINNs for moderate and high Reynolds number fluid flows.

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MS31

Global Sensitivity Analysis of a Hemodynamic Digital Twin in Post-Hepatectomy Liver Failure

Liver surgery is a crucial intervention for treating primary or secondary liver tumors, with partial hepatectomy being a common approach. However, the risk of Post-Hepatectomy Liver Failure poses a significant concern, often attributed to post-operative portal hypertension (PHT). This work outlines a global sensitivity analysis (SA) of a validated lumped-parameter model that simulates the whole-body hemodynamic response to partial hepatectomy, aiming to unravel the key factors influencing clinical outcomes, and specifically assessing the risk of PHT. The SA study focuses on essential input parameters, including heart elastances, resistances in various vascular components, and the fraction of the total liver mass to be resected. Driven by clinical necessities in evaluating patient status during hepatectomy, the analysis examines preoperative and post-operative variables such as portal vein pressure, portocaval gradient, systemic arterial pressure, cardiac output, and blood flows in the hepatic artery

and portal vein. Employing the Sobol indices method, the model outputs are constrained to physiological ranges using an innovative approach based on the polynomial chaos expansion method, reducing computational costs for a comprehensive physiological SA. The outcomes of this work highlight the crucial parameters influencing the hemodynamic model, distinguishing between significant and negligible measurements.

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MS32

Sequential Design for Multi-Fidelity Computer Experiments with Different Mesh Densities

This talk will deal with the surrogate modeling of computer experiments in the case of a scalar output dependent on input parameters. We are more specifically interested in computer experiments that involve the use of finite element methods with a real-valued tuning parameter that determines the fidelity of the numerical output. In these cases, integrating this fidelity parameter in the analysis enables us to make inference on fidelity levels that have not been observed yet. Such models have been developed and we aim to create a sequential design based on the Integrated Mean Square Prediction Error (IMSPE) to identify the best next design points across input parameters and fidelity parameter, while taking into account the computational cost associated with the fidelity parameter. We illustrate this methodology through synthetic simulations and applications to finite element analysis.

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MS32

Uncertainty Quantification in the Presence of Intrinsic Stochasticity for Multifidelity Discrete Fracture Network Simulations

Large-scale discrete fracture network (DFN) simulators are standard fare for studies involving the sub-surface transport of particles since direct observation of real world underground fracture networks is generally infeasible. While these simulators have seen numerous successes over several engineering applications, estimations on quantities of interest (QoI) such as breakthrough time of particles reaching the edge of the system suffer from a two distinct types of uncertainty. A run of a DFN simulator requires several parameter values to be set that dictate the placement and size of fractures, the density of fractures, and the overall permeability of the system; uncertainty on the proper parameter choices will lead to some amount of uncertainty in the QoI, called epistemic uncertainty. Furthermore, since DFN simulators rely on stochastic processes to place fractures and govern flow, understanding how this randomness affects the QoI requires several runs of the simulator at distinct random seeds. The uncertainty in the QoI attributed to different realizations (i.e. different seeds) of the same random process (i.e. at identical input parameter values) leads to a second type of uncertainty, called aleatoric uncertainty. We will discuss methods for attributing the uncertainty observed in the QoI to the epistemic uncertainty from each input parameter and to the aleatoric uncertainty, and review an application to DFN simulations.

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MS32

Distribution Regression for Bias Correction of Multifidelity Stochastic Simulators

Stochastic computer models are often deployed to simulate physical processes. Such simulators may exist at varying fidelities, with higher fidelities being more physically accurate but at an increased computational cost compared to biased, low-fidelity simulators. The underlying stochasticity suggests running ensemble simulations, which may be prohibitively expensive at high fidelities. In this work, we propose a functional data, distribution-on-distribution bias correction model which predicts high-fidelity distributional output from low-fidelity distributional output. Our model respects constraints on distribution-based functional data objects (e.g., PDFs / CDFs) through use of log quantile density (LQD) functions. In particular, we specify a Gaussian process (GP) model on a basis decomposition of LQD discrepancies, which allows known covariates from the low-fidelity simulation to inform the bias correction model. Furthermore, GPs enable uncertainty quantification through predictive distributions. We motivate our approach using particle transport simulations through multi-fidelity representations of subsurface fracture networks, which is critical in understanding gas seepage at the surface spurred by underground nuclear explosions.

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MS33

Integrating Machine Learning and Data Assimilation Algorithms for High Dimensional Dynamical Systems

Data Assimilation (DA) and Machine Learning (ML) methods are extensively used in predicting and updating high-dimensional spatial-temporal dynamics. Typical applications span from computational fluid dynamics to geoscience and climate systems. In recent years, much effort has been given in combining DA and ML techniques with objectives including but not limited to dynamical system identification, reduced order surrogate modelling, error covariance specification and model error correction. This talk will provide an overview of state-of-the-art research in this interdisciplinary field, covering a wide range of applications. The author will also present the unpublished work regarding efficient deep data assimilation with sparse observations and time-varying sensors. The proposed method, incorporating a deep learning inverse operator based on Voronoi tessellation into the assimilation objective function, is adept at handling sparse, unstructured, and time-varying sensor data.

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MS33

Uncertainty Quantification and Automatic Task Balancing of Bayesian Physics Informed Neural Networks for Inverse Problems in Reactive Flows

We present an efficient data-assimilation framework based on deep learning and integrating robust uncertainty quantification to address pore-scale reactive inverse problems, targeting both imaging data and physics-based constraints. This approach lies in a Bayesian Physics-Informed Neural Networks (BPINNs) formulation of multi-objective inverse problems involving the PDE constraints as tasks, for which we introduce a new method of automatic task balancing. This strategy establishes an adaptive weighting of the target distribution in a Bayesian context and ensures unbiased uncertainty quantification through an automatic weighting of the tasks in multi-objective problems. Task balancing is directly achieved by leveraging gradient information of the various objectives within the BPINNs framework, maintaining efficient computational costs. Our approach benefits from improved convergence and stability in contrast to conventional formulations, and eliminates the need for manual adjustment of critical weighting parameters. The adjusted weights also bring information on the task uncertainties and thus improve the reliability of the noise-related and model adequacy estimates. After demonstrating the effectiveness of this framework on data assimilation problems of various complexities, we apply it to pore-scale imaging of reactive inverse problems in porous media, to capture morphological uncertainties on the micro-porosity field and reliability ranges on the kinetic parameters.

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MS34

On Satellite Image Data Algorithms

High-resolution remote sensing images, while desirable for many applications requiring detailed feature extraction, e.g. pixel-wise segmentation tasks, are currently limited in their availability temporally and spatially due to limitations in technology and hardware costs. However, there is a growing number of publicly available lower-resolution satellite datasets with relatively high revisit times, e.g., Sentinel-2 data. Applying machine learning algorithms on lower-resolution images presents challenges, one of which is the potential for a decrease in the quality and certainty of the features extracted from the satellite images. In this talk, we discuss strategies and methods for two tasks: (1) change detection and (2) building and road segmentation in lower-resolution satellite images. This work was done by Mission Support and Test Services, LLC, under Contract No. DE-NA0003624 with the U.S. Department of Energy. DOE/NV/03624–1797.

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MS34

Quantifying Uncertainties in Limited-Angle Tomography: Applications to Dynamic Materials Science Experiments

We are interested in extracting information from dynamic materials science experiments where the primary data comes from (1) X-ray radiographs taken from two views and (2) photon doppler velocimetry (PDV) data. Tomographic reconstructions of the two-view radiographic images are powerful tools for interrogating the physics of dynamic materials science experiments. Since the tomographic reconstructions will inform fundamental research, uncertainty quantification plays a central role in qualifying the trustworthiness of experimental results. The uncertainty estimates from radiographic images depend upon a cascade of sources of error including the parametric uncertainty of the experimental setup, shot-to-shot variability of the X-ray machine, loss of information through digitization, assumptions of the underlying physics model used for inversion, uncertainty arising from the chosen computational reconstruction algorithm, etc. This work considers sources of uncertainty in density estimates alongside techniques for decreasing uncertainty, e.g., incorporating the experiments PDV data.

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MS34

Realistic Depictions of Knowledge from the Intersection of Uncertainty Quantification and Experiment Design

Modern machine learning methods represent the cutting edge in many analysis and data interpretation tasks; however, successfully applying these approaches to high-consequence problems remains challenging, largely owing to the difficulty producing consistent and defensible estimates of uncertainty associated with model outputs. Although there are methods to estimate aspects or components of uncertainty associated with data-driven learning, these estimates may be incomplete or inadequate for capturing and communicating the actual state of information associated with a models output and fail to answer relevant application questions. To effectively capture the interpretable knowledge produced by data-driven methods, we combine novel machine learning methods that emphasize native, sample-specific uncertainty quantification with numerical experiments. These experiments are designed to provide quantitative answers to questions or requirements, while simultaneously profiling our methods performance with various challenges and application constraints

and identifying edge cases. We illustrate these approaches using examples involving isotopic analysis of environmental and bulk irradiated nuclear reactor fuel samples for treaty verification, which requires analyzing the isotopic composition of reactor fuel material to identify the reactor of origin or estimate operation parameters to confirm or deny consistency with declarations made in international treaties.

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MS34

Computing and Communicating Uncertainty in AI-based Medical Imaging Applications for Healthcare Decision Making

AI-based Decision Support Systems (DSS) in the healthcare domain often aim to assist decision-makers such as radiologists in making high-stakes decisions. Incorrect AI-generated predictions can potentially mislead interpretation and analysis, leading to grave consequences for patient care and their quality of life. Among growing calls for Transparent and Responsible AI, Uncertainty Quantification (UQ) plays a critical role for calculating and communicating the confidence in AI model predictions. However, decision-makers often do not have the technical background to apply UQ-based methods and to fully grasp the implications of UQ results. In this talk, we discuss challenges for computing and communicating uncertainty in high-stakes application of AI-based medical imaging. We begin by introducing a computationally-efficient procedure to obtain Bayesian UQ for deep learning models. We then describe the utility of these UQ results for radiologists through uncertainty maps for MRI scans. Lastly, we adopt a cognitive psychology lens to describe how non-math savvy decision-makers utilize AI uncertainty information in their decision-making process.

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MS35

Sampling for Sparsity-Promoting Hierarchical Bayesian Models Using Prior Normalization

Recovering sparse generative models from limited and noisy measurements presents a significant and complex challenge. Given that the available data is frequently inadequate and affected by noise, it is crucial to assess the resulting uncertainty in the relevant parameters. Notably, this uncertainty in the parameters directly impacts the reliability of predictions and decision-making processes. In this talk, we explore the Bayesian framework, which facilitates the quantification of uncertainty in parameter estimates by treating involved quantities as random variables and leveraging the posterior distribution. Within the Bayesian framework, sparsity promotion and computational efficiency can be attained with hierarchical models with conditionally Gaussian priors and gamma hyperpriors. However, most of the existing literature focuses on the numerical approximation of maximum a posteriori (MAP) estimates, and less attention has been given to sampling methods or other means for uncertainty quantification. To address this gap, our talk will delve into recent advancements and developments in uncertainty quantification and sampling techniques for sparsity-promoting hierarchical Bayesian inverse problems.

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MS35

Generalized Sparsity-Promoting Solvers and Samplers for Hierarchical Inverse Problems

Bayesian hierarchical models have been demonstrated to provide efficient algorithms for finding sparse solutions to ill-posed inverse problems. The models typically employ a conditionally Gaussian prior model for the unknown, augmented by a hyper-prior governing auxiliary local variance parameters. Here, we generalize efficient point-estimation algorithms and convexity analysis for these models in three ways: (1) we generalize to sparsifying transformations possessing trivial kernels, (2) we allow treating the noise variance as a random variable which is made part of the inference procedure, and (3) we consider the context of Bayesian data fusion in which multiple data sources with distinct sensing modalities and noise characteristics must be synthesized. To provide partial uncertainty quantification, we detail a computationally efficient priorconditioned Gaussian sampling algorithm that is asymptotically exact. We demonstrate the performance of our methods on a suite of numerical examples.

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MS35

Bayesian Biomechanics: Exploration of Muscle Recruitment During Motion

Human motion is characterized by abundant redundancy: A given series of motions such as walking can be effectuated by different activation patterns of muscles, making it possible to operate in changing external or conditions or when impaired by disease or aging. A central question in biomechanics is to understand how, and based on which principles, the central nervous system chooses the muscle recruitment patterns, and how to characterize the uncontrolled manifold of activations that result essentially to the same movement. In this talk, Bayesian methods are employed to implement various prior distributions that correspond to different physiological assumptions, and MCMC sampling techniques are applied to characterize the corre-

sponding possible muscle recruitment patterns.

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MS36

Inexact Proximal Langevin Sampling

In order to solve tasks like uncertainty quantification or hypothesis tests in Bayesian imaging inverse problems, we often have to draw samples from the arising posterior distribution. For the usually log-concave but high-dimensional posteriors, Markov chain Monte Carlo methods based on time discretizations of Langevin diffusion are a popular tool. If the potential defining the distribution is non-smooth, these discretizations are usually of an implicit form leading to Langevin sampling algorithms that require the evaluation of proximal operators. For some of the potentials relevant in imaging problems this is only possible approximately using an iterative scheme. We investigate the behaviour of a proximal Langevin algorithm under the presence of errors in the evaluation of proximal mappings. We generalize existing non-asymptotic and asymptotic convergence results of the exact algorithm to our inexact setting and quantify the bias between the target and the algorithm's stationary distribution due to the errors. We show that the additional bias stays bounded for bounded errors and converges to zero for decaying errors in a strongly convex setting. We apply the inexact algorithm to sample numerically from the posterior of typical imaging inverse problems in which we can only approximate the proximal operator by an iterative scheme and validate our theoretical convergence results.

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MS36

Learning the Optimal Regularizer for Inverse Problems

Variational regularization is a well-established technique to tackle instability of inverse problems, and it requires solving a minimization problem in which a mismatch functional is endowed with a suitable penalty term. The choice of such a functional is a crucial task, and it usually relies on theoretical suggestions as well as a priori information on the desired solution. A promising approach to this task is provided by data-driven strategies, based on statistical learning theory. In this talk, I will consider linear inverse problems (associated with relevant applications, e.g., in signal processing and in medical imaging), and aim at learning the optimal regularization operator, in a suitable sense. I will first focus on the family of generalized Tikhonov regularizers, for which it is possible to prove theoretical properties of the optimal operator and error bounds for its approximation as the size of the sample grows, both with a supervised-learning strategy and with an unsupervised-learning one. Finally, I will discuss the extension to different families of regularization functionals, with a particular interest in sparsity-promotioning ones. This is based on joint work with G. S. Alberti, E. De Vito (University of Genoa), M. Lassas (University of Helsinki) and L. Ratti (University of Bologna).

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MS36

Bayesian Inference under Model Misspecification and Optimal Transport

In the context of inverse problems, Bayesian optimal experimental design (BOED) provides an optimization-based framework to choose sensor locations that yield the most informative observations. For the most common choices of objective functions in BOED, the resulting optimization criteria consists of some form of posterior variance minimization. In BOED, one often assumes that the parameter-to-observable map or 'forward model' that is used for inference is correct. In most real-world applications, however, the forward model is 'misspecified': it differs from the true forward model. Misspecification can lead to a biased posterior where the bias does not vanish in the limit of infinite data. In this case, the classical BOED criteria based on minimizing posterior variance become unsuitable. We propose a BOED framework that explicitly accounts for forward model misspecification, for linear Gaussian inverse problems. We use this framework to highlight the shortcomings of classical BOED for misspecified forward models, and propose some use-cases.

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MS37

Reverse Diffusion Processes for Bayesian Inference: Solving the Jacobi-Bellmann Equations with Tensor Trains

Sampling from probability densities is a common challenge in fields such as Uncertainty Quantification (UQ) and Generative Modelling (GM). In GM in particular, the use of reverse-time diffusion processes depending on the log-densities of Ornstein-Uhlenbeck forward processes are a popular sampling tool. These log-densities can be obtained by solution of a Hamilton-Jacobi-Bellman (HJB) equation known from stochastic optimal control. While this HJB equation is usually treated with indirect methods such as policy iteration and unsupervised training of black-box architectures like Neural Networks, we propose instead to solve the HJB equation by direct time integration, using compressed polynomials represented in the Tensor Train (TT) format for spatial discretization. Crucially, this method is sample-free, agnostic to normalization constants and may avoid the curse of dimensionality due to the TT compression. We provide a complete derivation

of the HJB equation's action on Tensor Train polynomials and demonstrate the performance of the proposed time-step-, rank- and degree-adaptive integration method on a nonlinear sampling.

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MS37

Quasi-Monte Carlo for Bayesian Optimal Experimental Design Problems Governed by PDEs

The goal in Bayesian optimal experimental design (OED) is to maximize the expected information gain for the reconstruction of unknown quantities in an experiment, by optimizing the placement of measurements. The objective function in the resulting optimization problem contains a high-dimensional integral with respect to the posterior distribution. In this talk, we will explore the use of tailored quasi-Monte Carlo methods to approximate these high-dimensional integrals efficiently in order to reduce the computational burden associated with Bayesian OED problems governed by partial differential equations. Numerical experiments are presented to assess the theoretical results.

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MS37

Stochastic Inverse Problems for PDEs with Discontinuous Coefficients

Detecting (stochastic) inclusions via limited observations in a setting modeled by a partial differential equation has various applications in the sciences. We present Bayesian inversion methods for the detection of stochastic (discontinuous) inclusions modeling heterogeneous media by observing the solution of an elliptic partial differential equation. After providing a general formulation for a variable stochastic setting, an efficient numerical approach is developed. A machine-learning-based method is employed to lower the computational complexity the high-dimensionality of the problem inherently brings. We approximate the solution operator of the partial differential equation with a deep neural network and present numerical results showcasing the computational benefit that can be achieved by our method. Quantifying the uncertainty associated with a point estimator for the posterior distribution derived via Bayesian methods remains challenging, especially if the parametrization of the inclusions is high-dimensional and sensitive. The Bayesian setup allows for rigorous uncertainty quantification which is essential given the ill-posed nature of an inverse problem. We present efficient techniques to quantify the uncertainty in the position and shape of the detected inclusions from (limited) measurements.

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MS37

Bayes for Parametric PDEs with Normalizing Flows

We approach the Darcy inverse problem in a Bayesian setting with multilevel normalizing flows. Normalizing flows are able to approximate complex posterior distributions, offering a robust framework for accurate parameter estimation and uncertainty quantification in the context of inverse problems. A bottleneck in training the normalizing flows is the availability of large sets of highly accurate solutions to the Darcy problem. To avoid the cost of solving the Darcy problem for many parameter fields, we use a multilevel neural network as a surrogate for the forward problem. The Kullback-Leibler (KL) divergence can then be minimized using the generated data. Furthermore, the surrogate model can be incorporated in the backward KL divergence. Furthermore, we leverage a decomposition of the solutions into a coarse grid approximation and finer grid corrections to build a multilevel normalizing flow with the advantage of a smaller network size and more efficient training.

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MS38

Discretization of Parameter Identification in PDEs using Neural Networks

We consider the ill-posed inverse problem of identifying a nonlinearity in a time-dependent PDE model. The nonlinearity is approximated by a neural network, and must be determined alongside unknown parameters and state. Proposing an all-at-once approach, we bypass the need for training data, and recover all unknowns simultaneously. Generally, approximation via neural networks can be realized as a discretization scheme, and training with noisy data can be seen as an ill-posed inverse problem. Therefore, we study discretization of regularization in terms of

Tikhonov and projected Landweber methods, proving convergence as discretization error and noise level tend to zero.

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MS38

Sparse Grid Approximation of Stochastic Parabolic PDEs: The Landau-Lifshitz-Gilbert Equation

We consider the Stochastic Landau-Lifshitz-Gilbert (SLLG) problem as an example of parabolic stochastic PDE (SPDE) driven by Gaussian noise. Beyond being a popular model for magnetic materials immersed in heat baths, the forward uncertainty quantification (UQ) task poses several interesting challenges that did not appear simultaneously in previous works: The equation is strongly nonlinear, time-dependent, and has a non-convex side constraint. We first use the Doss-Sussman transform to convert the SPDE into a random coefficient PDE. We then employ the Lvy-Ciesielski parametrization of the Wiener process to obtain a parametric coefficient PDE. We study the regularity and sparsity properties of the parameter-to-solution map, which features countably many unbounded parameters and low regularity compared to other elliptic and parabolic model problems in UQ. We use a novel technique to establish uniform holomorphic regularity of the parameter-to-solution map based on a Gronwall-type estimate combined with previously known methods that employ the implicit function theorem. This regularity result is used to design a piecewise-polynomial sparse grid approximation through a profit maximization approach. We prove algebraic dimension-independent convergence and validate the result with numerical experiments. If time allows, we discuss the finite element discretization and multi-level approximation.

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MS38

Numerical Linear Algebra Networks for Solving Linear Inverse Problems

We consider solving a probably ill-conditioned linear operator equation, where the operator is not modeled but specified via training pairs of the input-output relation of the operator. We derive a stable method for the solution of the operator equation, where an essential part is orthonormalization of input and output samples, respectively.

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MS38

Learning Theory for Importance Weighted Risk Minimization

Importance weighted risk minimization (IWRM) is one of the main methods for learning from unlabeled data (e.g., from new medical patient) using related labeled data following a different distribution (e.g., expert-annotated data from previous medical patient). In this work, we explore a link between the considered learning problem and the estimation of Radon-Nikodym derivatives in reproducing kernel Hilbert spaces. As a result, we provide convergence rates for regularized IWRM. This talk is based on (E.R. Gizewski, L. Mayer, B. Moser, D.H. Nguyen, S. Pereverzyev Jr, S.V. Pereverzyev, N. Shepeleva, and W. Zellinger., Applied and Computational Harmonic Analysis 57 (2022); W. Zellinger, S. Kindermann, and S.V. Pereverzyev. arXiv preprint 2307.16164 (2023)).

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MS39

A Comprehensive Study of Spike and Slab Priors for Structurally Sparse Bayesian Neural Networks

Network complexity and computational efficiency have become increasingly significant aspects of deep learning. Sparse deep learning addresses these challenges by recovering a sparse representation of the underlying target function by reducing heavily over-parameterized deep neural networks. Specifically, deep neural architectures compressed via structured sparsity (e.g. node sparsity) provide low latency inference, higher data throughput, and reduced energy consumption. In this talk, I will provide a detailed overview of the Bayesian sparse solutions using a suite of spike-and-slab priors to allow for automatic node selection during training. The use of spike-and-slab prior alleviates the need for an ad-hoc thresholding rule for pruning. In addition, we adopt variational inference including continuous relaxation of Bernoulli variables to circumvent the computational challenges of traditional Markov Chain Monte Carlo implementation. We empirically demonstrate the competitive performance of our models compared to

the baseline models in prediction accuracy, model compression, and inference latency.

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MS39

Probabilistic Neural Architecture Search for Uncertainty Quantification in Neural Networks

In this talk, we explore the significance of creating robust machine learning models with well-calibrated uncertainties, especially crucial for scientific applications. We delve into the Bayesian paradigm in probabilistic machine learning that provides a structured method for attaining robustness and understanding uncertainty through distributional estimates. We will introduce and discuss our UraeNAS approach, which merges probabilistic architecture and weight ensembling, focusing on both the weight and architectural space uncertainties in neural networks. This novel method relies on a refined posterior distribution, emphasizing a sparser super-network and progressively pruning less impactful operations for optimizing performance. The Bayesian framework facilitates versatile architecture and weight sampling, offering a diverse set of candidates and utilizing Bayesian model averaging to ensure more reliable predictions

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MS39

Classification Using Support Vector Machines with Uncertainty Quantification

Binary classification using machine learning is needed to address engineering problems such as identifying passing/failing parts based on measured features from aging hardware. In these classifications, providing the uncertainty of each prediction is essential to support engineering decision making. One popular classifier is the support vector machine (SVM). There are many variations, with the simplest being a linear division between two classes with a hyperplane. Kernel methods can be implemented for data that is not linearly separable. Adding the use of a loss function allows for control over misclassification in the training data. The many variants of SVMs and their tunable model parameters readily enable ensembling, which we use to represents model (epistemic)?uncertainty. SVMs also can be used to depict intrinsic uncertainty in the data, or aleatoric uncertainty. One of the major shortcomings of SVMs is that they make predictions indiscriminately over the entire prediction space, resulting in seemingly high-confidence predictions where there is no data. In this talk, we present one way around this by combining ideas from outlier-detection methods and SVMs, with the goal being to surround each class while simultaneously separating it from the other class. A unique representation of UQ results from this single-class SVM strategy is presented. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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MS39

Bayesian Neural Networks Predicting Aleatoric and Epistemic Uncertainties

In the realm of machine learning, uncertainties pose a challenge throughout the pipeline, ranging from data generation to model training. These uncertainties can be categorized into aleatoric uncertainty and epistemic uncertainty, where the former one stems from data and cannot be eliminated; the later one originates from the model and can be reduced . Bayesian neural networks (BNNs) have emerged as a promising approach to characterize uncertainties while the computational resources of training reliable BNNs are overwhelming. Furthermore, being capable of distinguishing aleatoric uncertainty and epistemic uncertainty is another challenge when performing inference with BNNs because they are usually entangled and difficult to separate from each other. In this talk, we give an overview of the essential theory on how to train and determine uncertainties from BNNs. We also share our insights on how to reasonably disentangle aleatoric and epistemic uncertainties. To evaluate the performance of selected BNNs, we conduct a series of comparative studies on different numerical problems. These studies aim to explore the strengths and limitations of different BNN methods in predicting Quantities of Interest, various types of uncertainties, and extrapolation capabilities. Based on the comparative studies, we report our finding by highlighting the different applicability of the methods considered and proposing a potential strategy for predicting heteroscedastic uncertainties.

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MS40

Bayesian Optimization with Bayesian Deep Kernel Learning

Bayesian optimization methods use a probabilistic surrogate model of the objective function, most commonly Gaussian processes. However, using a Gaussian process requires specifying a kernel. The choice of the kernel is critical for achieving good performance, but this choice is often challenging for practitioners. In this talk, we discuss using Bayesian deep kernel learning to automatically learn a kernel on the fly. Intuitively, this approach learns a distribution over embeddings over which a simpler kernel (such as a linear kernel) can be used effectively. We show that our method outperforms standard approaches using standard kernels as well as a non-Bayesian deep kernel learning approach in several synthetic and real-world test problems, including protein and nanophotonics design problems. We also show that Thompson sampling under this probabilistic model enjoys a sublinear regret guarantee.

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MS40

High-dimensional Bayesian Optimization

Bayesian optimization (BO) is a powerful paradigm for sample-efficient optimization of black-box objective functions and has been successfully used in many real-world scientific and industrial applications. However, even with recent methodological advances, the application of BO to problems with small evaluation budgets is generally limited to simple low-dimensional domains. In this talk, we introduce our new Sparse Axis-Aligned Subspace BO (SAASBO) method which is very sample-efficient and can handle search spaces with hundreds of tunable parameters. We show that SAASBO achieves excellent performance on several high-dimensional real-world problems, including optimizing a production-scale on-device natural language understanding model at Meta.

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MS40

Latent Space Bayesian Optimization for Machine-Assisted Drug Discovery

One natural framework for drug design problems is black-box optimization. For example, a biochemist might aim to design some object of interest (e.g. an antibody or molecule) which maximizes some objective function (i.e. its binding affinity to some useful protein). Typically, no mathematical form is available for this objective function, and it may be expensive to evaluate, making it a black box. Bayesian optimization (BO) is a popular machine learning method for solving black-box optimization problems. However, typical BO methods assume a continuous numerical search space, thus preventing them from being directly applied to search over structured, discrete objects such as molecules. Latent space Bayesian optimization (LS-BO) has recently emerged as a promising approach for optimizing over such search spaces. LS-BO utilizes a deep autoencoder model (DAE) to map the structured search space to a continuous latent space. This enables the use of standard BO techniques to perform the search for new molecules in the continuous latent feature space extracted by the DAE, rather than directly over the discrete space of molecules. In this talk, I will given an overview of LS-BO and discuss our recent work in improving current LS-BO methods for drug-design.

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MS40

Dirichlet Active Learning: A Scalable and Interpretable Method to Ensure Exploration and Exploitation for Labeling Data in Classification Tasks

We introduce Dirichlet Active Learning, a Bayesian-inspired approach to the design of active learning algorithms. This framework models the feature-conditional class probabilities as a Dirichlet random field and lends observational strength between similar feature vectors in order to calibrate this random field. This random field can then be utilized in learning tasks: in particular, we can use current estimates of mean and variance to conduct classification and active learning tasks. We demonstrate the applicability of this model to low-label rate graph learning by constructing "propagation operators' based upon graph Laplacians, and offer computational studies demonstrating the method's competitiveness with the state of the art. Finally, we provide rigorous guarantees regarding the ability of this approach to ensure both exploration and exploitation, expressed in terms of cluster exploration, distributional coverage, and increased attention to decision boundaries.

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MS41

Addressing Uncertainty in Manufacturing Engineering: Surrogate Models for Plastics Flow

Computer simulations are a widely used tool in computational science and engineering to, e.g., analyze the behavior of components or materials, enhance manufacturing processes with fast and accurate a-priori forecasts, or even control those processes during ongoing operation. With the help of these tools, we wish to make reliable assertions and predictions for one or more quantities of interest (QoI), also in the presence of uncertainty, e.g., in process conditions, material properties, or similar. Thus, methods from the field of Uncertainty Quantification (UQ) can enhance the quality of processes and products by augmenting the results for the QoI with quantified probability measures. We consider sampling-based UQ methods that usually require a great number of model evaluations. Thus, employing high-fidelity models may easily exceed available resources. Here, the usage of surrogate models, which are computationally cheaper, can provide a remedy. Therefore, we first follow the path of Model Order Reduction (MOR). In particular, we explore the benefits of intrusive MOR techniques and use Proper Orthogonal Decomposition (POD) with a subsequent Galerkin projection of the operators onto the constructed subspaces. As an alternative, we also investigate the advantages of Gaussian Process Regression (GPR) as a meta-model. Finally, the integration of the resulting surrogate models into a UQ setting is demonstrated for applications coming from polymer processing.

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MS41

Approximating the Smallest Eigenvalue of Large Hermitian Matrices That Depend on Parameters

We investigate the numerical solution of the global optimization problem

$$\lambda_{LB} = \min_{\mu \in \mathcal{D}} \lambda_{-1}(\mu), \tag{1}$$

where $\mathcal{D}$ is a compact subset of $\mathbb{R}^p$ and $\lambda_{-1}(\mu)$ denotes the

smallest eigenvalue of a parametric dependent hermitian matrix

$$A(\mu) := \sum_{l=1}^{\kappa} f_l(\mu) A_l \tag{2}$$

where $A_l : \mathbb{C}^n \to \mathbb{C}^n$ and $f_l : \mathcal{D} \to \mathbb{R}$ for $l = 1, ..., \kappa$ represent given hermitian matrices and real-analytic functions, respectively. Being able to solve in a fast and reliable way problem (1) is crucial in *projection Model Order Reduction*, in particular for the construction of reduced spaces through *greedy algorithms*, see Hesthaven & al. 2016. In general problems of type (1) come with two main challenges: 1) they are nonconvex and 2) they have an elevate computational complexity. To deal with these difficulties we develop an algorithm that, concerning 2), employs the *subspace* framework (Kangal & al. 2018) which enables to significantly *reduce the computational complexity*; concerning 1) it relays on `EigOpt` (Mengi & al. 2014). The proposed algorithm, under suitable assumptions, can be shown to be globally convergent.

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MS41

Exploiting Locality in Sparse Polynomial Approximation of Parametric PDEs

We consider the solution to an elliptic partial differential equation with coefficient and right-hand side depending smoothly but potentially highly nonlinearly on a parametric, function-valued input. When using a basis expansion to represent this input, using locally supported functions can improve the convergence rates of polynomial-based surrogates compared to globally-supported basis functions. As a notable case, we will see that this holds when the parametric input represents the shape of the domain and we are interested in a surrogate for the solution to the partial differential equation on a reference configuration. For this case, we consider different mappings to the reference configuration, showing that they all lead, theoretically and numerically, to higher convergence rates of Taylor-based surrogates when locally supported basis functions are used to represent the parametric shape.

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MS41

Model Order Reduction for Seismic Applications

Full waveform inversion to monitor changes in seismicity is a computationally expensive and challenging task. The latter is due to the fact that the discretization of the seismic wave equation can have millions of degrees of freedom. Moreover, aiming at estimating, for instance, the elastic structure at every grid point results in a large parameter space within the inverse problem. Model order reduction (MOR) techniques can help to speed up the computations, using low-dimensional models that capture the original system's important features. However, for large-scale wave propagation problems, constructing efficient reduced models is challenging as MOR methods can suffer from a slow decay of the Kolmogorov n-width for such problems, thus, requiring a large number of basis functions to reach the desired accuracy. In our work, we address the mentioned challenge as follows: We transform the problem to the Laplace domain, where we can exploit that the output of interest—the seismogram—is band-limited, such that we can avoid high frequencies; the latter would require many reduced basis functions for an accurate approximation. By targeting the construction of the reduced model to the seismogram, we obtain a rapidly converging reduced order approximation.

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MS42

Adaptive Low-Rank Approximation for the Optimization of Eigenvalue Problems in Nuclear Engineering

Low-rank approximation have recently been developed into an efficient method to solve high-dimensional problems. Their applications range from plasma physics and quantum mechanics to uncertainty quantification. In this talk, we will deal with the task of making such methods adaptive, which in many applications has the potential to dramatically increase their effectiveness. In particular, we will consider how approximations of different rank (and thus automatically generated models of different fidelity) can be used to aid mathematical optimization in cases where solving the forward problem on its own is already computationally expensive.

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MS42

Stochastic Finite Volume Method For Uncertainty Optimization of Gas Network Flows

Uncertain gas demand in pipeline networks originates from the intermittent nature of power loads and the interlinked gas generators. We develop a finite volume representation of uncertainty in solutions of hyperbolic partial differential equation systems on graph-connected domains with nodal coupling and boundary conditions. The representation is used to state the physical constraints in stochastic optimization problems subject to uncertain parameters. The method is based on the Stochastic Finite Volume (SFV) approach [Tokareva, S., Zlotnik, A., & Gyrya, V., Applied Mathematical Modeling, 2023], and can be applied for uncertainty management of gas flow over actuated transport networks. The method is tested on steady-state optimization of gas network flows subject to probabilistic constraints and the scalability of the method is examined for different test cases. The stochastic dynamic optimization gas flow problem with uncertain gas withdrawal is intro-

duced and derived using the SFV approach.

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MS42

Multilevel Strategy for Random Hyperbolic Conservation Laws

We discuss hyperbolic conservation laws with uncertain initial data. It is well known that deterministic hyperbolic conservation laws have discontinuities that arise in finite time. For random hyperbolic conservation laws, this can also lead to discontinuities in the stochastic direction. The interplay of the different scales makes it difficult to find an efficient method to approximate the stochastic moments. In this talk, we present a novel scheme by separating the spatial and stochastic scales and applying different grid adaptation strategies to the two different scales. For the spatial direction, we perform multiresolution-based grid adaptation on the stochastic moments while we perform multiresolution analysis with weighted thresholding in the stochastic direction. The resulting adaptive grids in each direction determine the resolution in the other direction and are adapted to the local structure of the corresponding solution. Thus, the interaction of the spatial and stochastic scales is considered. We illustrate our method with numerical examples and compare the results with Monte Carlo methods.

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MS43

Stabilizability of RHC for Linear Time-Varying Parabolic Equations under Uncertainty

In this talk, we investigate the stabilizability of linear time-varying parabolic equations with uncertain data using Receding Horizon Control(RHC). Within the RHC framework, the solution of an infinite-horizon optimal control problem is approximated through concatenating a sequence of finite-horizon ones in a receding horizon fashion. We address equations with random diffusion coefficients, explore both uniform and log-normal distributions, and employ finite-dimensional controls through indicator functions (actuators) in open spatial subsets. We analyze expected stabilizability and establish an upper bound on RHC failure probability with respect to the number of actuators and parameter choices.

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MS43

Risk-Averse PDE Constrained Optimization in the Presence of Data Corruption

A critical task when seeking to quantify and minimize the risk of rare, outlier events, such as structural failures or climate catastrophes, is to account for uncertainty in the underlying physical models. Uncertainty in physical systems is modeled with random variables, however, in practice there may be some nontrivial ambiguity in the underlying probability distribution from which they are sampled. This work describes an analytic frameworks that guarantee minimizers are robust to such ambiguities, as well as tensor decomposition methods to efficiently compute in the presence of high-dimensional uncertainty.

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MS43

Adaptive Gaussian Process Modeling for Trajectory Optimization with Model Inexactness

In many applications one must compute optimal trajectories from imperfect knowledge of the dynamics. For example, solving trajectory optimization problems for hypersonic vehicles requires the computation of lift and drag coefficients at many flight configurations. Determining these coefficients requires expensive high-fidelity computations using detailed representations of the hypersonic vehicle. This talk proposes the use of computationally inexpensive adaptive Gaussian process models constructed from high-fidelity samples to approximate the components of the dynamics that are expensive to evaluate. To reduce the effect of model errors on the optimal trajectory, the current Gaussian process model is updated as needed at the cost of evaluating the components of the dynamics at a small number of additional sample points. First, the optimal control problem is solved using the mean of the current Gaussian process model to represent the dynamics. Next, sensitivity analysis is combined with properties of the Gaussian process model, such as its variance, to determine whether the Gaussian process model needs to updated, and if so, at which samples the dynamics should be evaluated to update the Gaussian process model. This talk outlines our current model refinement procedure and demonstrates its performance on a trajectory optimization problem for a hypersonic vehicle with lift and drag models that are known,

but expensive to evaluate.

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MS43

Risk-averse Optimal Control of Random Elliptic VIs

We consider a risk-averse optimal control problem governed by an elliptic variational inequality (VI) subject to random inputs. By deriving KKT-type optimality conditions for a penalised and smoothed problem and studying convergence of the stationary points with respect to the penalisation parameter, we obtain two forms of stationarity conditions. The lack of regularity with respect to the uncertain parameters and complexities induced by the presence of the risk measure give rise to new challenges unique to the stochastic setting. We also propose a path-following stochastic approximation algorithm using variance reduction techniques and demonstrate the algorithm on a modified benchmark problem.

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MS44

Active Search for Bifurcations

Bifurcations mark qualitative changes of behavior in dynamical systems and can often lead to sudden transitions or catastrophic events. Accurately locating them is of paramount importance not just for deeper understanding of observed dynamic behavior, but also for designing efficient interventions. When the dynamical system at hand is complex, black-box or expensive to sample, standard numerical methods (e.g. continuation based) can become impractical. Here, we propose an Active Learning framework, where Bayesian Optimization is leveraged to discover saddle-node or Hopf bifurcations, from a judiciously chosen small number of vectorfield observations. Such an approach becomes especially attractive in systems whose exploration is resource-limited. It also naturally provides a framework for uncertainty quantification (aleatoric or epistemic), useful in systems with inherent stochasticity.

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MS44

Learning Interaction Laws in Particle and Agent-Based Systems

We consider systems of interacting agents or particles, which are commonly used for modeling across the sciences. Oftentimes the laws of interaction between the agents are quite simple, for example they depend only on pairwise interactions, and only on pairwise distance in each interaction. We consider the following inference problem for a system of interacting particles or agents: given only observed trajectories of the agents in the system, can we learn what the laws of interactions are? We would like to do this without assuming any particular form for the interaction laws, i.e. they might be any function of pairwise distances, or other variables, on Euclidean spaces, manifolds, or networks. We consider this problem in the case of a finite number of agents, with observations along an increasing number of paths. We cast this as an inverse problem, discuss when this problem is well-posed, construct estimators for the interaction kernels with provably good statistically and computational properties. We discuss the role of the geometry of the underlying space, in the cases of Euclidean space, manifolds, and networks, even in the case when the network is unknown. We also consider extensions to second-order systems, more general interaction kernels, stochastic systems, and to the setting where the variables (e.g. pairwise distance) on which the interaction kernel depends are not known a priori.

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MS44

Beware of Machine Learning Bearing Gifts in Numerical Analysis

Complex systems span multiple space and time scales, ranging from the microscopic scale where units interact, and the mesoscopic and macroscopic scales, where the emergent behaviour arises and the numerical analysis and control is usually sought. Thus, bridging systematically the scales constitutes an important, open challenge problem. If the coarse-variables are known, the Equation-free (EF) approach offers a numerical way bypassing the need to construct (global, generalizable) surrogate models, focusing on the numerical task we need to perform, and not on constructing a predictive and generalizable model. Another approach gaining power is the data-driven identification of surrogate machine learnng models for the solution of the inverse problem. For such machine learning models, the knowledge of an appropriate set of collective variables is necessary, while their approximation accuracy clearly depends very strongly on the quality of the training data. Last but not least, one confront with the curse of dimensionality. In this talk, I will present via some agent-based models the pros and cons that different machine learning approaches bear across scales and the need and importance for selecting the correct modelling approach for performing

the correct task, thus providing an overview, particularly with regard to applications, and suggest new venues for future research.

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MS44

Markov Chain Monte Carlo on Matrix Manifolds for Probabilistic Model Order Reduction

The purpose of Model Order Reduction (MOR) is to identify patterns and use them to decrease the number of dimensions of a problem as much as possible. Although often overlooked, it is important to quantify the uncertainty (UQ) associated with the reduction to trust the predictions made by the model. At the same time, incorporating domain knowledge into the UQ process is crucial, especially if data is sparse or noisy, which motivates the use of Bayesian statistics. This work aims to extend classical tools in model order reduction as well as more recent results in the field of optimisation on Riemannian manifolds to the probabilistic case, within the Bayesian framework. In particular, we present a method to sample from any given distribution defined on various matrix manifolds. In fact, matrix manifolds, in particular the Grassmann and the Siefel manifold, are used in model order reduction whenever linear subspaces of appropriate dimensions and orthogonality properties are sought. We present an adaptation of the Metropolis Adjusted Langevin Algorithm (MALA) that allows to draw samples from a posterior probability distribution of a random matrix defined on a matrix manifold. Results of the method will be shown, applied to the following problems: proper orthogonal decomposition (POD), active subspaces, and low-rank matrix completion.

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MS45

Dictionary-Based Model Reduction for State Estimation

We consider the problem of state estimation from m linear measurements, where the state to recover is an element of the manifold M of solutions of a parametric equation. The state is estimated based on Model Order Reduction (MOR). Variational approaches based on linear MOR, such as [Maday et al. A parameterized-background data-weak approach to variational data assimilation: Formulation, analysis, and application to acoustics. Int J Numer Methods Eng, 2015], yields a recovery error limited by the Kolmogorov m-width of M. To overcome this issue, piecewise-affine approximation was considered in [Cohen et al. Nonlinear Reduced Models for State and Parameter Estimation. SIAM-ASA J UNCERTAIN, 2022], where the affine space M is adaptively selected. In [Nouy et al. Dictionary-based model reduction for state estimation. Preprint, 2023], we propose a method relying on dictionary-based MOR, where a space is selected adaptively from a library generated by a dictionary of snapshots. The selection is made among a set of candidate spaces obtained from the path of LASSO problems. In the framework of parametric PDEs with affine parameterization, we provide an efficient offline-online decomposition based on randomized linear algebra [Balabanov et al. Randomized linear algebra for model reductionpart II: Minimal residual methods and dictionary-based approximation. Adv Comput Math, 2021.], that ensures efficient and stable computations while preserving guarantees.

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MS45

Structure-Preserving Adaptive Hyper-Reduction of Parametric Hamiltonian Systems

It is well known that model order reduction of non-linear dynamical systems does not typically result in significant speedups, since the computational cost of evaluating non-linearities still depends on the dimension of the full order problem. In the case of (parameterized) Hamiltonian systems, standard hyper-reduction techniques such as the empirical interpolation method (EIM) fail to preserve the geometric structure of the original problem, as the approximation of the non-linear Hamiltonian gradient is not a gradient in general. As an additional challenge, non-dissipative phenomena like transport-dominated problems and wave propagation do not possess a global low-rank structure, meaning that large approximation spaces are necessary to achieve even moderate accuracy. In order to address these issues, we present an adaptive, structure-preserving hyper-reduction scheme where the EIM basis and interpolation points are updated over time. A parameter sampling strategy is developed, so that the computational complexity of adapting the EIM space does not depend on the product of the full order dimension and the number of test parameters. We will also discuss how to update the dimension of both the reduced space and the hyper-reduction space to account for variations in the numerical rank of the state.

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MS46

Generative Neural Networks in Function Spaces

In this talk, I will discuss Continuous Generative Neural Networks (CGNNs), namely, generative models in the

continuous setting: the output of a CGNN belongs to an infinite-dimensional function space. The architecture is inspired by DCGAN, with one fully connected layer, several convolutional layers and nonlinear activation functions. In the continuous L^2 setting, the dimensions of the spaces of each layer are replaced by the scales of a multiresolution analysis of a compactly supported wavelet. We present conditions on the convolutional filters and on the nonlinearity that guarantee that a CGNN is injective. This theory finds applications to inverse problems, and allows for deriving Lipschitz stability estimates for (possibly nonlinear) infinite-dimensional inverse problems with unknowns belonging to the manifold generated by a CGNN. Several numerical simulations will be shown in order to illustrate and validate this approach.

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MS46

Parametric Shape Holomorphy of Boundary Integral Operators: Application to Operator Learning and Multi-fidelity Bayesian Inversion

We consider a family of boundary integral operators supported on a collection of parametrically defined boundaries. Firstly, we discuss the analytic or holomorphic dependence of said boundary integral operators upon the parametric variables, and illustrate the practical relevance of our findings by examining the sound-soft Helmholtz acoustic scattering problem and its frequency-robust boundary integral formulations. Next, we explore the relevance of this result in the context of data-driven techniques to forward and inverse uncertainty quantification in acoustic wave scattering. In particular, we explore the following approaches: (i) Data-driven learning of the parameter-to-solution map based on model order reduction techniques; and (ii) Multifidelity learning tailored to Bayesian inverse problems, with an emphasis on the small noise and large data limits. We present a comprehensive mathematical analysis of both approaches, leveraging the parametric holomorphy result. Finally, we provide numerical experiments showcasing the advantages of these data-driven techniques over traditional methods in terms of efficiency, accuracy, and scalability.

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MS46

Learning Sparsity-Promoting Operators for Inverse Problems

A common strategy to tackle instability in inverse problems is the use of regularizers, which are (families of) operators providing a stable approximation of the solution map. Alongside the classical model-driven regularization methods, which take advantage of prior information on the unknown solution, several data-driven methods have been proposed, which rely on large datasets and statistical learning techniques, leading to remarkable results. The most successful paradigms are based on a hybrid approach, combining the knowledge of the forward model and the information coming from training datasets to craft effective and reliable regularizers. In this context, I will discuss one approach that encodes, in a machine learning algorithm, some additional information about the desired solution: namely, its sparsity (with respect to an unknown basis). I will first set this problem in a general learning framework in infinite-dimensional spaces, which also provides a supervised strategy to approximate the optimal regularizer from a finite training sample. I will then show that the proposed technique can generalize from the training set: in particular, I will focus on sample error estimates, presenting an asymptotic error bound on the excess risk, and comparing it with previous results obtained for a different class of regularizers. This a joint project with G. S. Alberti, E. De Vito, M. Santacesaria (University of Genoa), M. Lassas (University of Helsinki), and T. Helin (LUT).

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MS47

Uncertainty Quantification for Deep Learning of Complex Systems

Modern science and engineering utilize physics-based models to inform decisions and guide design. In these settings, systems of interest are typically complex, exhibiting multiscale/-physics interactions and involving correlated/dependent and non-Gaussian variables. This talk presents two uncertainty quantification technologies for deep learning for physics-based models of complex systems. The first is Graph-Informed Neural Networks (GINNs), a strategy for incorporating domain knowledge into machine-learned surrogate models. This framework embeds expert knowledge, available data, and design constraints into a physics-based representation using probabilistic graphical models that provide a context for interpreting the surrogate's predictions, thereby enhancing defensibility. The second is Global Sensitivity Analysis (GSA) based on information theoretic dissimilarity measures. Our information-theoretic GSA provides a model-agnostic uncertainty quantification method for interrogating surrogates compatible with a wide range of black-box models. Effect rankings based on information-theoretic GSA assist in explaining surrogate predictions, thereby enabling deep-learning surrogates to close design loops for rapid simulation-based prototyping.

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MS47

Sampling with Mollified Interaction Energy Descent

Sampling from a target measure whose density is only known up to a normalization constant is a fundamental problem in computational statistics and machine learning. We present a new optimization-based method for sampling called mollified interaction energy descent (MIED), that minimizes an energy on probability measures called mollified interaction energie (MIE). The latter converges to the chi-square divergence with respect to the target measure and the gradient flow of the MIE agrees with that of the chi-square divergence, as the mollifiers approach Dirac deltas. Optimizing this energy with proper discretization yields a practical first-order particle-based algorithm for sampling in both unconstrained and constrained domains. We show the performance of our algorithm on both unconstrained and constrained sampling in comparison to state-of-the-art alternatives.

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MS47

Explicit Covariance Formulas and Estimation after Diagonal Transport

Consider the following transport problem: starting from a multivariate normal, transform each random variable one at a time with some (nonlinear) functions. We call this diagonal transport, and the resulting distribution is called nonparanormal. What are the moments of the nonparanormal distribution? In this talk, I'll give exact formulas for the mean and covariance, and discuss implications for independence and conditional independence properties. In some cases, the covariance entries obey a sort of heat equation, reminiscent of gradient flows in optimal transport.

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MS47

Transport, Variational Inference, and Diffusions

We explore the connections between optimal transport and variational inference, with a focus on forward and reverse time stochastic differential equations and Girsanov transformations.We present a principled and systematic framework for sampling and generative modelling centred around divergences on path space. Our work culminates in the development of a novel score-based annealed flow technique (with connections to Jarzynski and Crooks identities from statistical physics) and a regularised iterative proportional fitting (IPF)-type objective, departing from the sequential nature of standard IPF. Through a series of generative modelling examples and a double-well-based rare event task, we showcase the potential of the proposed methods.

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MS48

A Fully Parallelized and Budgeted Multi-Level Monte Carlo Method and the Application to Acoustic Waves

We present a novel variant of the multi-level Monte Carlo method that effectively utilizes a reserved computational budget on a high-performance computing system to minimize the mean squared error. Our approach combines concepts of the continuation multi-level Monte Carlo method with dynamic programming techniques following Bellmans optimality principle, and a new parallelization strategy based on a single distributed data structure. Additionally, we establish a theoretical bound on the error reduction on a parallel computing cluster and provide empirical evidence that the proposed method adheres to this bound. We implement, test, and benchmark the approach on computationally demanding problems, focusing on its application to acoustic wave propagation in high-dimensional random media.

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MS48

Software Design for Random Numbers and Quasi-Random Numbers

Software facilities to produce uniform random numbers and random variates from non-uniform distributions are key ingredients in modern computing. It is now recognized that a single generator that produces all the random numbers sequentially is not sufficient. We need multiple streams of random numbers that can run in parallel and act as independent generators. We should be able to safely use even billions of them. It is often convenient to also have multiple substreams within each stream. It should be possible to associate any stream with an arbitrary probability distribution to construct a non-uniform generator. In case we want to try quasi-Monte Carlo for an application, it should be easy to make a stream produce the quasirandom numbers (randomized or not)of our choice without changing the code of our simulation model. Such facilities are offered in the SSJ library (Stochastic Simulation in Java, https://github.com/umontreal-simul/ssj). I will explain how they are designed and integrated, give justifications, say what improvements we should add, and sketch out how I would do it in other languages.

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MS48

User-Friendly Link of Simulators to Lagun Platform: Applications to Real Problems of Uncertainty Quantification and Optimization

Lagun is an open-source platform dedicated to the explo-

ration and analysis of small datasets collected from experiments or expensive simulation models. Intended for non-expert users in computer experiments and uncertainty quantification, it is coded in R shiny to provide an interactive and user-friendly interface. In this talk, we will focus on Lagun's ability to connect any simulator that can be run on local or remote machines. This functionality allows active learning methods to be run for sensitivity and uncertainty analysis, or optimization based on simulated results. Monitoring and visualization tools are provided for on-the-fly verification and analysis of the simulations-based on-going procedure. Several real examples will be illustrated.

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MS48

Fast Gaussian Process Regression and Quasi-Monte Carlo in Julia

Gaussian process regression, or kriging, is a method for high dimensional interpolation which has gained popularity thanks to the ability to encode assumptions about the underlying simulation into the covariance kernel and the ability to quantify prediction uncertainty. A significant drawback is that fitting a kriging model to n data points typically costs $O(n^3)$ as it is required to solve a system involving the $n \times n$ Gram matrix of pairwise covariance kernel evaluations. Hickernell and Jagadeeswaran show in their 2019 and 2022 papers on fast automatic Bayesian cubature that when one has control over the design of numerical experiments then specially chosen sampling locations and matching covariance kernels yield structured Gram matrices for which we can complete all necessary computations in $O(n \log n)$. Specifically, lattice and digital sequences from Quasi-Monte Carlo paired with matching kernels yield circulant and block-Toeplitz Gram matrices respectively. We have extended the cubature rules implemented in QMCPy to surrogate modeling with support for noisy observations and derivative information. We present methods and Julia software for fitting these fast kriging models in $O(n \log n)$, including software to generate Quasi-Monte Carlo point sets. The software is demonstrated by modeling the solution process of a PDE with random coefficients.

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MS49

Forward Uncertainty Evolution of General Random Differential Equation Systems

Random Differential Equations are a versatile and flexible approach to studying and quantifying uncertainty evolution in differential equation-governed systems. The most important feature that can be computed is the First Probability Density Function (1-PDF). Although there are various methods for its computation, we have focused on using the Liouville, or Continuity, equation (see [T.T. Soong, Random Differential Equations, Thm. 6.2.2], [F. Santambrogio, Optimal Transport for Applied Mathematicians, Ch. 4]). The equation, in its conservative form, can be written as:

$$\partial_t f + \nabla_{\mathbf{x}} \cdot [\mathbf{g} f] = 0,$$

where f is the 1-PDF and $\mathbf{g}$ is defined at the RDE. If $\mathbf{g}$ is smooth, it can also be written as:

$$\partial_t f + \mathbf{g} \cdot \nabla_{\mathbf{x}} f = -f \nabla_{\mathbf{x}} \cdot \mathbf{g},$$

We will show the relationship between RDE systems and the Liouville equation and how it relates to another widely used method for quantifying uncertainty in RDEs. We will also briefly discuss our computational techniques for computing its solution. Finally, we will show some of our latest research, applying these theoretical findings to attractive real-world mathematical models.

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MS49

Uncertainty Quantification of Dynamical Systems

In this talk I shall provide an overiew on recent progress to merge dynamical systems techniques with forward UQ. In classical dynamics the goal is to understand the phase space structure of a nonlinear system with a focus on invariant sets such as equilibria, periodic orbits or invariant manifolds. Furthermore, these objects depend on parameters so one has to study their bifurcations under parameter variation. Yet, this approach has so far almost always negelected parametric uncertainty that is inherent in most models. To address this issue, we have to overlay/combine the approach of UQ with classical dynamics computations such as bifurcation point analysis, pattern computation and/or numerical continuation. I shall outline for several low-dimensional ODE models, how this can be accomplished and illustrate the additional information we gain by having a dynamical view of phase space with a probabilistic structure.

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MS49

Sensitivity Analysis for Bifurcations in Random Ordinary Differential Equations

How does parameter uncertainty affect nonlinear dynamics? A dynamical system can undergo a critical transition, that is tipping from its current stable state to a drastically different one, when a control parameter is varied and crosses a critical threshold value. This transition can happen suddenly and is oftentimes irreversible. To prevent systems from tipping, a better understanding of such events is needed. We approach these tipping phenomena through the lense of bifurcation theory, which provides a mathematical framework for the creation and loss of equilibria as well as changes in their stability properties under variation of a deterministic control parameter. This theory is well-developed for deterministic dynamical systems disregarding uncertainties. However, real-world applications induce the need to take uncertainties in model parameters into account. In this talk, I will introduce a novel combination of sensitivity analysis and bifurcation theory allowing for a quantification of parameter uncertainties in complex models. I will illustrate our methodology for a conceptual climate model of the Atlantic Meridional Overturning Circulation, which is one of the identified earth system tipping elements, and present numerical results on its tipping behaviour.

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MS49

Stochastic Dynamical Indicators: Theory and Applications

The talk will introduce the concept of stochastic dynamical indicators, their theoretical foundations and some examples of applications to astrodynamics. Stochastic dynamical indicators are scalar quantities that allow one to directly study the effect of uncertainty on the evolution of dynamical systems. It will be shown how the indicators can be used to identify regions of practical stability under the effect of parametric uncertainty and how the value of the indicators relates to the Lagrange stability of the dynamical system. It will also be shown that stochastic indicators reduce to more familiar chaos indicators, in some particular cases, and can be used to identify Lagrange coherent structures. Finally the talk will introduce the idea of diffusion structures as the counterpart of Lagrange coherent structures in the case of parametric uncertainty.

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MS50

Embracing Uncertainty in Optimization: Machine Learning-Based Approaches for Marine Propeller Optimal Design

Marine propeller design has long fascinated scholars and engineers. Their designs directly affect vessel performance, fuel efficiency, and emissions. Nonetheless, designing efficient, reliable, cost-effective, and environmentally compliant propellers in varying conditions while reducing noise and vibration poses significant challenges. Marine propellers often operate under uncertain conditions, including inflow, rate of revolutions, and manufacturing tolerances. Traditional designs ignoring uncertainty may result in less-than-ideal real-world performances. The computational intensity to pinpoint these uncertainties can be overwhelming, even with mid-fidelity tools like Boundary Element Methods (BEM). To overcome this problem, surrogate models can be used to simplify the vast calculations required to assess design uncertainties. Consequently, Simulation-Based Design Optimization becomes a tangible alternative to standard methods. In our study, we juxtapose traditional and robust designs for a standard propeller, considering operational uncertainties. Using BEM, we fine-tune machine learning-based surrogate models. We then validate our models using BEM solvers, showcasing the enhanced performance of our robust design methodology.

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MS50

From Epistemic Uncertainty Quantification to Design Space Dimensionality Reduction in Structural Optimization via Parametric Model Embedding

Simulation-driven optimization allows to identify innovative design solutions and new concepts. High-fidelity prime-principle-based models and solvers provide accurate design performance, while optimization algorithms drive

the search for the desired optimal solution. This process is usually computationally very costly especially if global optimization is sought after, as (i) high-fidelity models/solvers are computationally expensive and (ii) many design performance evaluations are needed in global optimization, facing the so-called curse of dimensionality. One possible remedy is to leverage the epistemic uncertainty associated with the design-problem solution and reduce the design space dimensionality using a suitably defined Karhunen-Love expansion. Recently, the authors have developed a methodology, so-called parametric model embedding (PME), for the design-space dimensionality reduction of parametric models in shape optimization for hydrodynamic applications. The objective of the present talk is to discuss the extension of PME to structural optimization problems. Here, the PME data matrix uses structure-relevant features and is demonstrated for the design-space dimensionality reduction of a 40 ft generic prismatic planing hull (GPPH) slamming in waves at high speed.

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MS50

Adaptive Multi-Fidelity Surrogate Modeling for the Uncertainty Quantification of Ship Performance

In the design of marine/ocean vessels, the uncertainty associated with the operational conditions and the design variables is a need-to-know information to achieve robust design configurations. The increase of the available computational power allows to use, with a high computational cost, high-accuracy physics-based solvers to obtain accurate predictions of innovative designs in extreme operating conditions. However, such technological improvement faces two main limitations: i) the number of designs and/or conditions that can be investigated is limited by the high computational cost; ii) high performance systems are not available to most of the designers. To overcome such limitations, multi-fidelity (MF) approaches can be used to reduce the number of high-accuracy simulations required to perform uncertainty quantification (UQ) of the design affected by operational and/or geometrical uncertainty. Specifically, MF approaches allow to combine solvers with different accuracies to reduce the overall cost of the UQ process. The objective of this work is the investigation of the performance of the MF method Multi-Index Stochastic Collocation (MISC) when applied to the UQ of the performance of the DTMB 5415. Operational and geometrical variables uncertainties are considered. The simulations are performed with the in-house linear potential flow solver WARP. A comparison of MISC against its single-fidelity counterpart will be provided and discussed.

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MS50

Uncertainty Quantification of An Optimized Configuration of a Multiple Propeller Combination

A large-scale wind tunnel model conceived to investigate the aerodynamic and acoustic performance of distributed electrical propulsion (DEP) on aircraft wings in high lift conditions was investigated in previous work [A. Visingardi, M. Barbarino and D. Quagliarella, Aerodynamic and Acoustic Design Optimization of a Multiple Propeller Combination for Distributed Electrical Propulsion, in WCCM-APCOM2022]. The optimization process aimed to obtain the best possible improvements in Noise and Aerodynamic performance by modifying the propellers layout of the Wing-DEP wind tunnel model. A multi-objective, multi-point design approach was adopted based on evolutionary computing. The present work aims at studying the uncertainty sources, both in terms of working conditions and manufacturing tolerances, that influence the DEP wing performance. This preliminary parametric analysis aims to identify, using the analysis of variance, the main dependencies and interactions of the parameters that describe the uncertainty sources [D. Quagliarella and E. Iuliano, UQ Sensitivity Analysis and Robust Design Optimization of a Supersonic Natural Laminar Flow Wing-Body, in 'Uncertainty Management for Robust Industrial Design in Aeronautics']. Indeed, the proper setup of a robust design problem requires correctly identifying these sensitivities and their reciprocal influence. The research work is carried out in the framework of the VENUS EU-funded project GA N. 886019.

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MS51

Comparing Monte Carlo Sampling Algorithms Using a Benchmark Bayesian Inverse Problem

We present the details of a prototypical benchmark for Bayesian inverse problems in which we seek to identify the posterior probability distribution of a discretized coefficient in an elliptic partial differential equation. We then use this benchmark to compare a number of simple and not-so-simple Monte Carlo sampling algorithms to assess how they perform using this benchmark as a test case that has many of the same features as real-world inverse problems.

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MS51

PyOED: An Open Source, Backend-Agnostic, Bayesian OED Toolbox for Rapid Development

PyOED is a highly extensible scientific package that enables developing and testing model-constrained optimal experimental design (OED) for inverse problems. Specifically, PyOED aims to be a comprehensive Python toolkit for model-constrained OED. The package targets scientists and researchers interested in understanding the details of OED formulations and approaches. It is also meant to enable researchers to experiment with standard and innovative OED technologies with a wide range of test problems (e.g., simulation models). Thus, PyOED is continuously being expanded with a plethora of Bayesian inversion, data assimilation (DA), and OED methods as well as new scientific simulation models, observation error models, priors, and observation operators. These pieces are added such that they can be permuted to enable testing OED methods in various settings of varying complexities. Although the tradeoff for extensibility is scalability, this is precisely PyOED's mission: to enable rapid development and benchmarking of OED methods with minimal coding effort and to maximize code re-utilization. We will showcase a brief demonstration on PyOED's layout and provide a set of test cases and tutorials to demonstrate how the package can be utilized.

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MS51

hIPPYlib: An Extensible Software Framework for Large-Scale Inverse Problems Governed by PDEs

hIPPYlib is an extensible software framework for the solution of large-scale deterministic and Bayesian inverse problems governed by partial differential equations with possibly infinite-dimensional parameter fields, which are high-dimensional after discretization. hIPPYlib overcomes the prohibitive nature of Bayesian inversion for this class of problems by implementing state-of-the-art scalable algorithms for PDE-based inverse problems that exploit the structure of the underlying operators, notably the Hessian of the log-posterior. The fast and scalable (with respect to both parameter and data dimensions) algorithms in hIPPYlib allow to address critical questions in applying numerical simulations to real-world problems: 1) How does uncertainty propagate from the inputs to the outputs of a mathematical model (forward UQ)? 2) How to infer model parameters from data with quantified uncertainties (Inference)? 3) How/Where/When to collect data to further reduce uncertainty (Optimal design of experiments)? 4) How to mitigate uncertainties in the final outcome (Decision making under uncertainty)? In summary, not only hIPPYlib makes advanced algorithms easily accessible to domain scientists, but it is also a teaching tool that can be used to educate researchers and practitioners who are new to inverse problems and the Bayesian inference framework.

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MS51

Deep Inverse: a PyTorch Library for Solving Inverse Problems with Deep Learning

Despite the ever-increasing research effort in the field of imaging inverse problems, most deep learning-based algorithms are built from scratch, are hard to generalize beyond the specific problem they were designed to solve, and the results reported in papers are often hard to reproduce. In order to tackle these pitfalls, I will present Deep Inverse (https://deepinv.github.io/), an open-source PyTorch library for solving imaging inverse problems with deep learning. The library covers most of the steps in modern imaging pipelines, from the definition of the forward sensing operator to the training of unfolded reconstruction networks in a supervised or self-supervised way. In this talk, I will focus on the uncertainty quantification methods included in the library, such as Langevin sampling with plug-and-play priors and diffusion models.

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MS52

Climate Model Integration and Downscaling: Spatial Models with Quantified Uncertainty

We propose a statistical downscaling method to produce fine-resolution climate projections. A multivariate spatial statistical model is developed to jointly analyze high-resolution remote sensing data and coarse-resolution climate model output. With a basis function representation, the resulting model can achieve efficient computation and describe potentially nonstationary spatial dependence. We implement our method to produce downscaled sea surface temperature (SST) projections over the Great Barrier Reef region from CMIP6 Earth system models. Compared to the state of the art, our method reduces the mean squared

predictive error substantially and produces a predictive distribution enabling holistic uncertainty quantification analyses.

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MS53

A Unified Reduced-Order-Modelling Framework for Prediction and Uncertainty Quantification in Parametric Nonlinear Systems

In their most recent formulation, Digital Twins are recast as closed-loop systems comprising a digital and physical counterpart in constant interaction. A main enabler to such a scheme are Reduced Order Models (ROMs), which deliver accurate simulators yet fast to compute. In this context, our work couples Variational Autoencoders (VAEs) with projection-based ROMs to address the challenge of response prediction in parameter-dependent nonlinear systems. Our approach initiates with a library of local ROMs, each representing a training realization of the parameters. In prediction mode, we utilize the decoder portion of a suitably trained VAE to relate the parameters to a suitable local subspace. The proposed ROM assumes no knowledge of the actual parameter values during prediction mode; instead, it utilizes a conditional latent space as a generative model, which can infer the local basis corresponding to features extracted from the monitored response. In parallel, an auxiliary regression task uses the latent space and the extracted features to perform the parameter estimation task. Thus, the derived ROM retains the physical insights of a projection-based strategy, allowing the integration of the dynamics while uncertainty quantification on the response estimates is injected via the probabilistic treatment of the VAE representation. These components lead to an efficient and generalized low-order representation with high utility for structural health monitoring tasks.

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MS53

First-principle-like reinforcement learning of nonlinear numerical schemes for conservation laws

In recent years, machine learning has been used to design numerical schemes such as flux limiters. However, existing methods either use direct numerical simulation data or rely on existing flux limiters for training, which raises concerns about the schemes' ability to generalize across varying physical equations and spatial dimensionsa standard capability of traditional CFD numerical schemes. We propose a novel multi-agent reinforcement learning (MARL) method for the universal design of nonlinear numerical schemes for hyperbolic conservation laws, which are typically challenged by spurious oscillations near discontinuities. Leveraging fundamental CFD principles without empirical parameters or reference data, our MARL approach automatically balances accuracy and numerical dissipation. It can generalize to different initial conditions, physics (governing equations), meshes, and even spatial dimensions, just like traditional CFD schemes. To our knowledge, it is the first machine-learned scheme trained on 1D Burger's equations that generalizes to 2D Euler equations.

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MS54

Covariance Operator Estimation in the Small Lengthscale Regime

Covariance matrix and covariance operator estimation are fundamental tasks in statistics and play an important role in many branches of science and engineering. In this talk, we will focus on covariance operator estimation via thresholding. For random fields with approximately sparse covariance operators, we establish non-asymptotic bounds on the estimation error in terms of the sparsity level of the covariance and the expected supremum of the field. We prove that thresholded estimators enjoy an exponential improvement on the sample complexity compared with the standard sample covariance estimator if the field has a small correlation lengthscale. As an application of the theory, we study thresholded estimation of covariance operators within ensemble Kalman methods.

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MS54

Long-Term Dynamics of Multiscale Systems with Data-Driven Model Closure

Model closures based on data have attracted a lot of interest in recent years due to the rapid developments in machine learning. Multiscale dynamical systems are approximated with reduced-order models that are augmented with closures, or parameterizations, inferred from data. It has been demonstrated for a variety of systems that data-driven closures improve the finite-time predictions generated by the hybrid model (reduced-order model plus closure). The lead time at which predictions remain accurate can vary substantially between different approaches for learning the closure from data. Furthermore, capturing the correct long-timescale behavior, such as transitions between different regimes or metastable states, using closures trained on short segments of model trajectory data is nontrivial. I will discuss some recent results on these issues.

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MS54

Quantifying Extreme Events in Complex Systems via Sample Path Large Deviations

Rare and extreme events are notoriously hard to handle in any complex stochastic system: They are simultaneously too rare to be reliably observable in numerics or experiment, but at the same time often too impactful to be ignored. Traditional rare events estimates based on large deviation theory only yield the exponential tail scaling of rare events. In this talk, I will discuss algorithms that improve on this limitation, yielding sharp quantitative estimates of rare event probabilities from a single computation and without fitting parameters. The applicability of this method to high-dimensional systems, such as extreme waves or liquid thin-film rupture, will be discussed.

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MS54

CNN Surrogate Inspired Score-based Generative Inverse Solver for Mechanics Problems Under Complex Priors

In the realm of inverse estimation for partial differential equation (PDE)-governed models, such as hyperelastic models, challenges arise when estimating infinite-dimensional functions within the computational domain. The ill-posed nature of such problems necessitates leveraging prior information to establish well-posedness. In most existing inverse solvers, the prior distribution is assumed to be of Gaussian or Laplace forms, which are often an oversimplification to many practical scenarios. In case the prior is complex and the likelihood model, via the forward model, is computationally expensive, drawing the sample from such posteriors can be computationally intractable, especially when the unknown is high-dimensional. In this work, firstly, to deal with complex and unknown prior distributions, we introduce an efficient sampling method, namely, a score-based diffusion model. This model combines a score-based generative sampling tool with a stochastic differential equation (SDE)-driven noising process and its corresponding reverse SDE-driven denoising process for iterative sample generation in accordance with the posterior distribution. Secondly, to expedite the simulation of non-parameterized PDEs and enhance the generalization capacity, we introduce a physics-informed convolutional neural network surrogate for the forward model. Finally, numerical experiments highlight the efficacy of the proposed approach.

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MS55

The Horseshoe Prior for Edge-Preserving Bayesian Inversion

In many large-scale inverse problems characterization of sharp edges in the solution is desired. In the Bayesian approach to inverse problems, edge-preservation is often achieved using Markov random field priors based on heavy-tailed distributions. Another strategy, popular in sparse statistics, is the application of hierarchical shrinkage priors. An advantage of this formulation lies in expressing the prior as a conditionally Gaussian distribution depending on heavy-tailed distributed hyperparameters. In this presentation, we revisit the shrinkage horseshoe prior and introduce its formulation for edge-preserving settings. We discuss a Gibbs sampling framework to solve the Bayesian inverse problem. Applications from imaging science show that our computational procedure is able to compute sharp edge-preserving posterior point estimates with reduced uncertainty.

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MS55

Iterative Sample Refinement for Sparsity Promoting Bayesian Hierarchical Models

In this talk, we present a method for sampling from sparsity promoting Bayesian hierarchical models where the parameters are conditionally distributed like a regularized Gaussian distribution. For ordinary Gaussian distributions, samples can be obtained by solving a randomized linear least squares problem; If combined with a Gibbs sampler, then convergence guarantees exist even if the randomized linear least squares problem is solved inaccurately. However, if sparsity promoting regularization is added to the randomized linear least squares problem, then these guarantees do not hold. We propose a method focused on iteratively refining existing samples instead of obtaining more samples. This method can be shown to convergence

and the computations can be easily parallelized. We show the benefits of this method for the sparse regularized case and discuss whether it is beneficial for the unregularized case.

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MS55

Rough Feature Estimation via Alpha-Stable Priors and Mixture Models

The estimation of rough features can be done either by specialised non-Gaussian priors or hierarchical models. In this talk, we review certain techniques for constructing such estimation algorithms. We first consider alpha-stable random models constructed with finite differences, and show that the resulting posteriors are multimodal, heavy-tailed and high-dimensional. Then we consider the construction of these priors via Bayesian neural networks and scale-mixture models. As an alternative we us mixture of Gaussian process models, where the rough features are modelled through different GPs. For this algorithm, we need to estimate also all GP parameters, thus requiring joint state and parameter estimation, for which we use SMC^2, that is two nested sequential Monte Carlo algorithms.

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MS55

Towards Dimension Reduction of Bayesian Inverse Problems with Neural Network Priors

We study Bayesian inverse problems where the unknown target function is represented with neural networks. Priors based on neural networks with random weights/biases have been employed due to their discretization-independent property and potential ability to capture discontinuities. The focus is on obtaining the posterior distribution of these weights/biases, which proves challenging due to its high dimensionality and multimodal nature. To address this issue, we explore gradient-based dimension reduction methods to improve computational efficiency and network interpretability. We share initial findings in this direction through a simple numerical example.

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MS56

Moment Based Point Spread Function Hessian Approximation for Large Scale Ice Sheet Inverse Problems

Antarctic ice sheet discharge is predicted to be a dominant driver of global sea level rise over the next century. However, ice sheet flow dynamics depend on the basal sliding friction field, which cannot be measured directly and must be inferred by solving a large scale inverse problem governed by a Stokes partial differential equation (PDE). Existing state-of-the-art methods for solving the inverse problem are based on low rank approximation of the prior preconditioned data misfit Hessian in the inverse problem. This is extremely computationally costly because the numerical rank of the data misfit Hessian is large. We reduce this cost by approximating the Hessian using a new moment-based point spread function (PSF) method. Existing methods require thousands of PDE solves to approximate the Hessian, while our new method requires only twelve.

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MS56

Connecting Large-Eddy Simulations of Stratocumulus Clouds to Predator Prey Dynamics via Feature Based Inversions

How our climate changes is heavily influenced by Earths energy budget. Stratocumulus clouds have a great effect on Earths energy budget because (i) they can reflect sunlight; and (ii) they cover about thirty percent of our planet. It is thus important to understand and model stratocumulus clouds and in this talk, we make connections between two very different models. The first model is a large eddy simulation (LES), which is a cloud resolving 3D atmospheric simulation that is computationally expensive to run. The second model is a scalar delay differential equation (DDE), which is trivial to run and interprets the interactions of precipitation and cloud as a predator (rain) and prey (cloud) system. We connect these two models by estimating parameters of the predator-prey model from LES that reflect a variety of meteorological conditions. We rely on a feature-based approach to parameter estimation and numerically solve the problem using an affine invariant ensemble sampler. The result of our computations is

a map of meteorological conditions to the parameter space of the predator-prey model. Interestingly, we discover a strong relationship between the nondimensional parameters of the DDE when exposed to various meteorological conditions from LES. These findings support the models ability to represent aspects of stratocumulus clouds, which is needed if one were to use it to parameterize stratocumulus clouds in Earth system and climate models.

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MS56

Operator Learning to Enable Atmospheric Source Inversion

In complex large-scale systems such as climate, important effects are caused by a combination of confounding processes that are not fully observable. The identification of sources from observations of the system state is vital for attribution and prediction, which inform critical policy decisions. Surrogate models may enable the many-query algorithms required for source identification, but training challenges arise from high dimensionality of the state and source compounded by limited ensembles of costly model simulations. The influence of auxiliary processes adds an additional layer of uncertainty that further confounds source identification. We discuss the use linear and nonlinear dimension reduction methods within surrogate modeling approaches for flow maps trained on an ensemble of simulations obtained by varying sources. We then utilize the surrogate models in a Bayesian framework to identify sources from observations via optimization using limited data in a high-variability environment.

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MS56

Randomized Physics-Informed Machine Learning Method for Uncertainty Quantification in High-Dimensional Inverse Problems

We propose a randomized optimization algorithm for uncertainty quantification (UQ) in high-dimensional inverse problems. Our method represents states and parameters of partial differential equations (PDEs) with truncated conditional Karhunen-Love expansions (CKLEs), which by construction respect measurements of the said variables. The maximum a posteriori (MAP) solution of the inverse problem is formulated as a minimization problem over CKLE coefficients where the objective/loss function is the sum of the norm of PDE residuals and a Tikhonov regularization term. The MAP formulation is known as the physics-informed CKLE (PICKLE) method. Uncertainties in the inverse solution are quantified in terms of the joint probability density function (PDF) of CKLE coefficients. This PDF is sampled from the randomized MAP minimization problem, which is formulated by adding zero-mean Gaussian perturbations in the PICKLE objective function. We call this approach the randomized PICKLE method or rPICKLE. We test rPICKLE for low- (15 dimensional) and high-(1000) dimensional inverse problems. For the low-dimensional case, we demonstrate that rPICKLE generates samples from the correct posterior via comparison with the Hamiltonian Monte Carlo (HMC) method. For the high-dimensional case, we find that rPICKLE still produces the correct posterior distribution while HMC fails to converge in a reasonable amount of time.

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MS57

Accounting for Uncertainties in the Land Friction Coefficient in Tsunami Modelling with Multi-Level Bayesian Quadrature

Future simulations of tsunamis are crucial for coastal engineering and urban planning. The land cover roughness is a very influential parameter in the numerical simulations of tsunami inundations, but it is actually a rather uncertain parameter. Hence one needs to develop approaches that include this uncertainty in such simulations. We propose here to regard the land cover roughness as a nuisance parameter, integrating out the nuisance parameter and accounting for uncertainty. We employ an efficient probabilistic numerical method, multilevel Bayesian Quadrature (MLBQ), to deliver this uncertainty quantification, making use of a mix of low and high resolution modelling to reduce computing costs as well. We use an end-to-end physical and numerical modelling to simulate the entire process, starting from the earthquake source. We compute outputs of momentum flux, a more valid quantity than flow height or velocity to represent forces on buildings. We illustrate our approach on future tsunamis for Sumatra, a seismically active region, where we are able to compute the probabilty distributions of local impact for a large tsunami source. Such approaches can be adopted the future for improved probabilistic hazard and risk assessments by combining these uncertainties with source uncertainties.

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MS57

Active Learning for a Recursive Non-Additive Emulator in Multi-Fidelity Computer Experiments

Computer simulations have become essential for analyzing complex systems, but high-fidelity simulations often come with significant computational costs. To tackle this challenge, multi-fidelity computer experiments have emerged as a promising approach that leverages both inexpensive but less accurate data and costly but highly accurate data, enhancing both the accuracy and efficiency of the analysis. In this paper, we introduce a novel and flexible statistical model, the Recursive Non-Additive (RNA) emulator, that integrates the data from multi-fidelity computer experiments. Unlike conventional multi-fidelity emulation approaches that rely on an additive auto-regressive structure, the proposed RNA emulator recursively captures the relationships between data with different fidelity levels using Gaussian process priors without making the additive assumption, allowing the model to accommodate more complex data patterns. Importantly, we derive the posterior predictive mean and variance of the emulator, which can be efficiently computed in a closed-form manner, leading to significant improvements in computational efficiency. Additionally, based on this emulator, we introduce an active learning strategy that optimizes the balance between accuracy and computational costs and guides the selection of the fidelity level and input locations for the next simulation run. We demonstrate the effectiveness of the proposed approach in a suite of synthetic examples and a real-world problem.

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MS57

A Bayesian Neural Network Approach to Multi-Fidelity Surrogate Modeling

This talk deals with the surrogate modeling of computer code results that can be evaluated at different levels of accuracy and computational cost,called multi-fidelity. We propose a method combining Gaussian process (GP) regression on low-fidelity data and a Bayesian neural network (BNN) on high-fidelity data, see [1]. The novelty, compared with the state of the art, is that uncertainties are taken into account at all fidelity levels. The proposed approach is then compared with several multi-fidelity GP regression methods on different examples. [1] Kerleguer, Baptiste, Claire Cannamela, and Josselin Garnier. "A Bayesian neural network approach to multi-fidelity surrogate modeling." International Journal for Uncertainty Quantification 14.1 (2024) pp. 43-60

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MS57

Greedy Multiscale Surrogates for Uncertainty Quantification

We discuss here a scheme for constructing surrogates of complex physical systems based on a greedy approach to selecting a set of multiscale basis functions. We apply it to problems from debris flow and combustion models. Our analysis of the method proves convergence of the surrogate and our results show performance comparable or superior to classical Gaussian process regression.

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MS58

Uncertainty-Aware Null Space Networks for Data-Consistent Image Reconstruction

Reconstructing an image from noisy and incomplete measurements is a central task in several image processing applications. In recent years, state-of-the-art reconstruction methods have been developed based on recent advances in deep learning. Especially for highly underdetermined problems, maintaining data consistency is a key goal. However, for such approaches to be used in safety-critical domains such as medical imaging, the network reconstruction should not only provide the user with a reconstructed image, but also with a certain level of confidence in the reconstruction. In order to meet these two key requirements, this talk will build on the work of [C. Angermann, S. Gppel, and M. Haltmeier, M. Uncertainty-Aware Null Space Networks for Data-Consistent Image Reconstruction, submitted (2023). https://arxiv.org/abs/2304.06955], we combine deep null space networks with uncertainty quantification. Evalua-

tion of the proposed method includes image reconstruction from undersampled Radon data and accelerated MRI reconstruction on the fastMRI dataset.

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MS58

Multigrid Monte Carlo Revisited

In this talk, I revisit the multigrid Monte Carlo (MGMC) method proposed by Goodman and Sokal [Goodman and Sokal, (1989) Multigrid Monte Carlo method. Conceptual foundations], a random sampler analogue of deterministic multigrid solvers. MGMC accelerates random samplers, such as Gibbs samplers, by drawing on insights from numerical analysis. The primary focus of this talk is to provide theoretical support. We discuss a grid-size-independent convergence theory for MGMC, applicable to general Gaussian random variables. This theory demonstrates that the first two moments, which fully characterize the Gaussian distribution, converge exponentially to their target values at a uniform rate. Additionally, we examine the exponential decay of autocorrelations in the generated samples. Furthermore, we extend the application of the MGMC method to address the important scenario of sampling posterior Gaussian distributions conditioned on noisy data.

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MS58

Universal Lattice Algorithm for Function Approximation in Uncertainty Quantification

We present an algorithm to approximate periodic functions that does not need to know the smoothness, and uses rank-1 lattice points. Rank-1 lattice points are characterised by a generating vector which in turn determines the quality of the approximation. We propose a component-by-component (CBC) construction to construct a generating vector for function approximation without prior information on smoothness parameters. This means the resulting generating vector can be used for any smoothness. In the application of uncertainty quantification, it leads to almost the same convergence rate as previous lattice algorithms except for some logarithmic factors.

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MS60

Posterior Sampling via Sliced MMD Flows with the Negative Distance Kernel

Maximum mean discrepancy (MMD) flows suffer from high computational costs in large scale computations. We show that MMDs with Riesz kernels coincide with the MMD of its sliced version. As a consequence, the computation of gradients of MMDs can be performed in the one-dimensional setting. A simple sorting algorithm can be applied to reduce the complexity from $O(MN + N^2)$ to $O((M + N)\log(M + N))$ for two measures with M and N support points. For the implementations, we approximate the gradient of the sliced MMD by using only a finite number P of slices and show that the resulting error has complexity $O(\sqrt{d/P})$, where d is the data dimension. These results enable us to train generative models by approximating MMD gradient flows by neural networks even for image applications. By approximating the joint distribution of ground truth and observations, we use them for posterior sampling and conditional generative modeling. The posterior sampling is used for uncertainty quantification in inverse problems, in particular superresolution, computerized tomography and image inpainting.

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MS60

Canonical Variates in Wasserstein Metric Space

In this study, we address the classification of instances each represented by a distribution in a vector space, rather than by a single point. We employ the Wasserstein metric to measure distances between distributions and then apply distance-based classification algorithms such as k-nearest neighbors, k-means, and pseudo-mixture modeling. Our focus is on dimension reduction in the Wasserstein metric space for enhanced classification. We introduce a novel approach grounded in the principle of maximizing Fisher's ratio. This ratio is defined as the quotient of between-class variation to within-class variation. The directions in which this ratio is maximized are termed discriminant coordinates or canonical variates axes. In practice, we define both

between-class and within-class variations as the average squared distances between pairs of instances, with the pairs either belonging to the same class or to different classes. An iterative algorithm is developed, which alternates between optimal transport and maximization steps within a vector space. We empirically investigate the algorithm's convergence and demonstrate through experiments that our dimension reduction method significantly improves classification. Additionally, our approach achieves superior performance compared to common algorithms on vector representations extracted from distributional data and exhibits robustness against variations in distributional representations of data clouds.

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MS60
Calibration of the Bass Local Volatility Model

The fitting problem is a classical challenge in mathematical finance about finding martingales that satisfy specific marginal constraints. Building on the Bass solution to the Skorokhod embedding problem and optimal transport, Backhoff, Beiglbck, Huesmann, and Kllblad propose a solution for the two-marginal problem: the stretched Brownian motion. Notably rich in structure, this process is an Ito diffusion and a continuous, strong Markov martingale. Following a similar approach, Conze and Henry-Larbordre recently introduced a novel local volatility model. This model, rooted in an extension of the Bass construction, is efficiently computable through a fixed-point scheme. In our presentation, we reveal the fixed-point scheme's intricate connection to the stretched Brownian motion and analyse its convergence. Moreover, we discuss an alternative computational method based on gradient flows on the Wasserstein space. This presentation is based on joint work with Beatrice Acciaio, Julio Backhoff, Antonio Marin, and Walter Schachermayer.

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MS60
Covariance Alignment with Optimal Transport

Dataset or feature alignment is a longstanding problem appearing in many areas including computer vision, natural language translation, and biostatistics. Here we show how a novel type of alignment problem arises in the matching of untargeted biological data where the concentrations of unlabeled biological molecules (features) are recorded over a collection of samples or patients. Partnering with biologists at the International Agency for Research on Cancer (IARC), we develop a practical and efficient tool for untargeted dataset alignment to be used in laboratory settings. Our approach aligns feature covariance matrices between datasets using the celebrated Gromov-Wasserstein (GW) algorithm from optimal transport. Motivated by the success of our approach, we investigate the statistical complexity of Gromov-Wasserstein for aligning empirical covariance matrices. Remarkably, we find that the GW algorithm achieves the same minimax optimal rates for this problem as a (quasi) maximum likelihood estimator, proving that it is statistically competitive. These results offer a new challenging setting for graph matching of Wishart (covariance) matrices and the first statistical rates of estimation for the Gromov-Wasserstein algorithm.

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MS61
Reduced Subgrid-Scale Terms for Turbulence Modelling

It is well known that the wide range of spatial and temporal scales present in turbulent flow problems represent a computational bottleneck, which must be circumvented by a coarse-graining procedure. The effects of the unresolved fluid motions enter the coarse-grained equations as an unclosed subgrid scale (SGS) term. Despite the coarse graining procedure, the SGS term still contains a high number of unclosed (and therefore unknown) degrees of freedom.
To decrease the degrees of freedom we switch our attention to capturing spatially-integrated quantities of interest (QoIs). Examples of such QoIs include climate-like statistics of the full model, for instance the global energy of the system. We show that if we restrict our interest to these small QoI, we do not need a SGS term with a large number of unclosed degrees of freedom. Instead, we can derive a ROM, that strikes a balance between physical insight and data-driven modelling, and which significantly reduces the amount of training data that is needed to model the remaining (small) unclosed component. This small remaining component is then the only part for which we construct a surrogate model via machine learning.
We derive the new ROM for two-dimensional turbulence in a doubly periodic square domain, and show that it produces the same statistics for our quantities of interest as the exact (full-field) SGS term, which is extracted from a high-resolution reference model.

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MS61
Reduced-Order Moment Closure Models with Random Batch Method for Complex Multiscale Systems

Nonlinear turbulent phenomena in complex multiscale dynamic systems are ubiquitous in many science and engineering problems. Effective modeling methods and efficient computational analysis in such processes remain a grand challenge and have significant social impacts in pressing issues. The capability of using imperfect statistical and stochastic reduced-order models to capture crucial statistics in turbulent systems is investigated. A much simpler and theoretically tractable modeling framework is pro-

posed using high-order stochastic-statistical moment closure enabling efficient ensemble prediction of leading-order statistical moments and probability density functions. To address challenges associated with closely coupled spatio-temporal scales in turbulent states and expensive large ensemble simulation for high-dimensional complex systems, we introduce efficient computational strategies using the random batch method. It is demonstrated that crucial principal statistical quantities in the most important large scales can be captured efficiently with accuracy using the reduced-order model in various dynamical regimes of the flow field with distinct statistical structures. Finally, various numerical experiments are performed showing effectiveness of the proposed models for a wide range of real-world applications in prediction, uncertainty quantification, and data assimilation.

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MS61

A Statistical Pod Approach for Feedback Control in Fluid Dynamics

Hamilton-Jacobi-Bellman (HJB) equation plays a central role in optimal control and differential games, enabling the computation of robust controls incfeedback form. The main disadvantage for this approach depends on the so-called curse of dimensionality, since the HJB equation and the dynamical system live in the same, possibly high dimensional, space. In this talk I will consider feedback boundary optimal control problems arising from fluid dynamics and their reduction by the means of a Statistical Proper Orthogonal Decomposition (SPOD) method. The Proper Orthogonal Decomposition (POD) is a well-known technique in the Model Order Reduction community used to reduce the complexity of intensive simulations. The SPOD approach is characterized by the introduction of stochastic terms in the model (e.g. in the initial condition or in the boundary conditions) to enrich the knowledge of the Full Order Model, useful for the definition of a more reliable controlled reduced dynamics. In the offline stage of the method we consider different realizations of the artificial random variables and we compute the corresponding optimal trajectory via the Pontryagin Maximum Principle (PMP), which will form our snapshots set. Afterwards, we construct the reduced basis and we consider the corresponding reduced dynamical system. Finally, I will show its effectiveness on the optimal control of the incompressible Navier-Stokes equation in a backward step domain.

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MS62

Multilevel Quadrature Rules for Optimization Problems under Uncertainty

In this talk, we consider the minimization of the expected value of a functional constrained by a random elliptic partial differential equation. One common approach to solve such problems is to discretize a-priori the probability space by replacing the continuous expectation with a Monte Carlo or Quasi Monte Carlo approximation. Since the computational cost grows with the number of quadrature nodes, several techniques have been proposed in the last years to ease the computational burden, including sparse grids and multilevel Monte Carlo methods. However, the methods proposed have the drawback of involving negative quadrature weights which may lead to the loss of the convexity of the continuous optimization problem. We therefore propose a novel and different approach to use general multilevel quadrature formulae to solve optimal control problems under uncertainty, while preserving the properties of the continuous optimization problem. We conclude by showing the efficacy through numerical experiments on nonlinear problems.

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MS62

A Tensor-Train Stochastic Finite Volume Method for Uncertainty Quantification

The stochastic finite volume (SFV) method has shown great promise as a non-intrusive PDE solver for uncertainty quantification. However, in many relevant applications, the dimension of the stochastic space can make traditional implementations of the SFV method infeasible or impossible due to the so-called curse of dimensionality. To obviate the curse of dimensionality, we evolve a tensor-train decomposition of the solution space. This necessitates a novel reformulation of the well-known cell based WENO reconstruction procedure resulting in a global reconstruction. The global WENO reconstruction allows us to efficiently compute flux terms, while previously implemented tensor-train quadrature rules are used to compute expectations.

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MS63

Numerical Solution of An Optimal Control Problem with Probabilistic and Almost Sure State Constraints

In this talk, we discuss optimization problems subject to random state constraints, where we distinguish between the chance-constrained case and the almost sure formulation. We highlight some of the difficulties in the infinite-dimensional setting, which is of interest in physics-based models where a control belonging to a Banach space acts on a system described by a partial differential equation (PDE) with random inputs or parameters. We study the setting in which the obtained state should be bounded uniformly over

the physical domain with high probability, or even probability one. For the numerical example, we use a model with a random elliptic PDE, where the randomness is induced by the right-hand side. For the chance-constrained setting, this structure allows us to obtain an explicit representation for the Clarke subdifferential of the probability function; this is possible using the spherical radial decomposition of Gaussian random vectors. This formula is used for the numerical solution in a discretize-then-optimize approach. For the almost sure setting, we use a Moreau-Yosida regularization and solve a sequence of regularized problems in an optimize-then-discretize approach. The solutions are compared, providing new insights for the development of further algorithms.

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MS63

Numerical Methods for State Constraints in PDE-Constrained Optimization under Uncertainty

State-constraints in PDE-constrained optimization under uncertainty are both theoretically as well as numerically much less understood than their deterministic counterparts. We investigate several modelling choices and associated optimization algorithms. First, we discuss our experience with a Moreau-Yosida-based quadratic penalty approach that allows a direct application of a semismooth Newton method after approximating the underlying probability measure with a sample-based empirical approximation. We contrast these results with an online stochastic approximation method that uses a (degenerate) reformulation of the state constraint as a scalar expectation constraint. We analyze this algorithm in the continuous setting under the assumption that we may perform periodic restarts. This leads to probabilistic convergence rates for optimal values and feasibility. As part of the numerical results, we provide a post-optimization analysis via a Kolmogorov-Smirnov test of the distributions of the random objective and constraint functional.

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MS63

Sample Size Estimates for Risk-Neutral Semilinear PDE-Constrained Optimization

The sample average approximation (SAA) approach is applied to risk-neutral optimization problems governed by semilinear elliptic partial differential equations with random inputs. After constructing a compact set that contains the SAA critical points, we derive nonasymptotic sample size estimates for SAA critical points using the covering number approach. Thereby, we derive upper bounds on the number of samples needed to obtain accurate critical points of the risk-neutral PDE-constrained optimization problem through SAA critical points. We quantify accuracy using expectation and exponential tail bounds. Numerical illustrations are presented.

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MS64

A Random Neural Network and Differential Geometry Based Method for the Detection of Extreme Events Precursors

Extreme events in economics, in climate, in health science and in engineering are those dynamical scenarios that may well lead to definitive changes that may break or permanently change coping mechanism. To develop a data-driven way to detect the onset of such an event is of high importance. We will show here that since feature selection is an extremely important step in such a goal, it can well be understood by a sufficiently rich neural network, even a partially trained such network, using concepts from high dimensional projection, especially when some prior knowledge of how certain differential geometry issues are relevant upon onset of extreme events in complex dynamical systems.

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MS64

Physics Informed Random Projections Neural Networks for the Numerical Solution of DAEs

We address the numerical solution of nonlinear stiff Differential Algebraic Equations (DAEs) via a novel adaptive physics-informed machine learning (PIML) approach based on Random Projections Neural Networks (RPNN). The method is a numerical assisted one that tackle the computational burst commonly associated with PIML schemes. It involves an efficient computation of the unknown weights between the hidden and output layer, with Gauss-Newton and sparse QR decomposition with L^2 regularization for medium to large-scale systems. The internal weights and biases were parsimoniously selected, and once and for all a priori fixed, via an extensive optimization based on the bias-variance trade-off decomposition. Furthermore, to handle stiffness and sharp gradients, we address an adaptive step-size scheme and a continuation method for providing good initial guesses for the Newton iterations. We assessed the performance of the scheme through eight benchmark problems, including three index-1 DAEs problems

and five stiff ODEs problems. For the first time, we demonstrated that a machine learning approach can compete with, and even outperform, established flagship of numerical analysis such as ode23t and ode15s from the Matlab ODE suite. Additionally, we compared it against the DeepXDE physics informed deep learning library, showing that our numerical-assisted machine learning scheme is much faster for the same numerical approximation accuracy.

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MS64

Slow Invariant Manifolds for Model Reduction of Systems of ODEs via Physics Informed Machine Learning

We introduce a Physics-Informed Machine-Learning (PIML) framework to approximate Slow Invariant Manifolds (SIMs) of stiff system of ODEs, for providing functionals of SIMs in an explicit form, thus facilitating the construction and numerical integration of reduced order models (ROMs). We consider two classes of stiff systems: (i) singularly perturbed systems characterized by explicit timescale splitting which is expressed by a perturbation parameter ϵ, and (ii) the more general form of slow-fast dynamical systems. The proposed scheme performs model reduction on the basis of Geometric Singular Perturbation Theory, by solving the invariance equation (IE). For the solution of IE, two neural network structures are considered; namely feedforward neural networks (FNNs), and random projection neural networks (RPNNs). Symbolic, numerical and automatic differentiation is used for the computation of the gradients required for the learning process. We assess the efficiency of the PIML method via a number of benchmark problems, demonstrating that the SIM approximations provided by the proposed PIML scheme are of equivalent, or even higher accuracy, than those provided by other traditional GSPT-based methods. Interestingly, in contrast to other GSPT-based methods, the PIML scheme is shown to be unaffected by the magnitude of the perturbation parameter; a result suggesting it employment in systems where the timescale gap is not that big, but still ROMs can be constructed.

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MS64

Next Generation Equation-Free Computations for Complex Systems

We present a data-driven computational framework, for the numerical bifurcation analysis and robust control of the emergent dynamics of complex systems, bridging, the Equation-free machinery, with nonlinear manifold learning and control theory. The Next-Generation EF approach obviates the need to learn from data surrogate deep-learning models, that introduce biases in the analysis. For our illustration, we apply the method to control the emergent unstable traveling waves of an agent-based model of traffic dynamics.

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MS65

Neural Surrogates for Fast and Scalable Bayesian Optimal Experimental Design

We address the solution of large-scale Bayesian optimal experimental design (OED) problems governed by partial differential equations (PDEs) with infinite-dimensional parameter fields. The OED problem seeks to find sensor locations that maximize the optimality criteria such as A-optimality, D-optimality, and expected information gain (EIG) in the solution of the underlying Bayesian inverse problem. These criteria are computationally prohibitive for large-scale PDE-based OED problems. We introduce fast and scalable algorithms to solve such problems based on Laplace and low-rank approximations, derivative-informed neural network surrogates, and a new swapping greedy optimization method. These algorithms exploit the geometry, smoothness, and intrinsic low-dimensionality of the parameter-to-observable map using only a small and dimension-independent number of PDE solves.

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MS65

Multiple-Fold Cross Validation for Model Selection in Universal Inversion

We consider large-scale linear inverse problems tackled in the framework of Universal Inversion (Traveletti 2023), where underlying input fields are endowed with prior distributions combining Gaussian Processes and linear trends in basis functions. While for prescribed basis functions and GP covariance kernels, Universal Inversion has the advantage of delivering a GP posterior with efficiently implementable posterior mean and covariance, in practice it is generally not straightforward how to specify these prescribed functions. We focus on the choice of basis functions and on how multiple-fold cross validation can be used as a tool to investigate the potential generalization abilities of resulting models. We are in particular interested in how the way to design the folds affects model comparisons, and numerically investigate this on a volcano gravimetry test case as well as on related artificially generated data sets.

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MS65

Modern Bayesian Experimental Design

Bayesian experimental design (BED) provides a powerful and principled information-theoretic framework for optimizing the design of experiments. However, its deployment often poses substantial computational challenges that can undermine its practical use. In this talk, we will outline how recent advances have transformed our ability to overcome these challenges and thus utilize BED effectively. We will discuss techniques aimed at making BED more practical for real-world applications, including methods for enabling online deployment and enhancing robustness to misspecifications of the underlying Bayesian model.

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MS65

Hierarchical and Nested Sampling for Optimal Experimental Design

Experimental design is an essential topic in engineering and science. Acquiring relevant information about processes and environments is paramount nowadays. Such cases include, among others, recording weather patterns, measuring traffic density, and tracking industrial process parameters. These data, once obtained, provide input for predictive modeling and process optimization. Experimental design allows us to optimize the locations of sensors to achieve the best estimates and minimize uncertainties, especially for real, noisy measurements. For instance, determining exactly how many sensors to use and their optimal location has significant implications for the reliability and value of the information obtained. We present hierarchical UQ techniques for computing the Expected Information Gain. These techniques are non-intrusive to facilitate their combination with existing simulation codes, drastically reducing the overall development costs. The actual sampling is flexible, allowing for using Monte Carlo, Quasi Monte Carlo, or Sparse Grids. Our formulation considers nuisance parameters, lowering the additional computational expenses using a Laplace approximation. We demonstrate the use of this methodology and the associated gains with numerical examples. Additionally, we show the impact of nuisance error on the optimal design.

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MS66

Towards Trustworthy Foundation Models for Weather and Climate

In this talk, I will present ClimaX, a flexible and generalizable deep learning model for weather and climate science that can be trained using heterogeneous datasets spanning different variables, spatio-temporal coverage, and physical groundings. ClimaX extends the Transformer architecture with novel encoding and aggregation blocks that allow effective use of available compute while maintaining general utility. The pre-trained ClimaX can then be fine-tuned to

address a breadth of climate and weather tasks, including those that involve atmospheric variables and spatio-temporal scales unseen during pretraining. Compared to existing data-driven baselines, we show that this generality in ClimaX results in superior performance on benchmarks for weather forecasting and climate projections, even when pretrained at lower resolutions and compute budgets. Towards the end of the talk, I will present ClimateLearn, our open-sourced library to standardize machine learning for climate science promoting transparency and reproducibility at large.

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MS66

Scalable Steering of Large Language Models Using Probabilistic Programs

Large language models are inherently probabilisticbut the probabilities they compute rarely reflect calibrated uncertainty about the task at hand. This is particularly true after reinforcement learning from human feedback, which can improve the reliability of the model but can also make it overconfident. In this talk, Ill propose an alternative approach to solving tasks reliably and with appropriate uncertainty using language models. The key idea is to specify the task at hand as a posterior inference problem in a language model probabilistic program, and then to replace standard decoding algorithms with sequential Monte Carlo (SMC) inference. For a computational cost similar to that of beam search, SMC can steer smaller pre-trained LLMs (e.g., the 7b-parameter Llama 2) to outperform GPT-4 on a variety of constrained generation tasks, both in terms of reliability (producing acceptable solutions) and calibration/coverage (accurately sampling the distribution of acceptable solutions). To effectively scale SMC for language models, we present a probabilistic programming library, LLaMPPL, for concisely specifying new generation tasks as language model probabilistic programs, and automating efficient, batched SMC for any language model in the HuggingFace model repository.

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MS66

DecodingTrust: Assessing Trustworthiness and Risks of Generative Models

Generative Pre-trained Transformer (GPT) models have exhibited exciting progress in capabilities, capturing the interest of practitioners and the public alike. Yet, while the literature on the trustworthiness of GPT models remains limited, practitioners have proposed employing capable GPT models for sensitive applications to healthcare and finance - where mistakes can be costly. To this end, this work proposes a comprehensive trustworthiness evaluation for large language models with a focus on GPT-4 and GPT-3.5, considering diverse perspectives - including toxicity, stereotype bias, adversarial robustness, out-of-distribution robustness, robustness on adversarial demonstrations, privacy, machine ethics, and fairness. Based on our evaluations, we discover previously unpublished vulnerabilities to trustworthiness threats. For instance, we find that GPT models can be easily misled to generate toxic and biased outputs and leak private information in both training data and conversation history. We also find that although GPT-4 is usually more trustworthy than GPT-3.5 on standard benchmarks, GPT-4 is more vulnerable given jailbreaking system or user prompts, potentially due to the reason that GPT-4 follows the (misleading) instructions more precisely. Our work illustrates a comprehensive trustworthiness evaluation of GPT models and sheds light on the trustworthiness gaps

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MS66

Epistemic Foundation Models: Progress and Open Challenges

Machine learning models and humans both have complex inner states. This talk will cover recent advances that enable better understanding of each type. First, I'll discuss recent interpretability work that enables humans to extract understandable and controllable hidden states from models. Next, I'll present work on using language models to interactively elicit and understand nebulous human goals and preferences. Finally, I'll discuss the connections between these two streams of work and their applications to safe and robust machine learning models.

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MS67

An Optimal Control Perspective on Diffusion-Based Generative Modeling Leading to Robust Numerical Methods

This talk establishes a connection between generative modeling based on SDEs and three classical fields of mathematics, namely stochastic optimal control, PDEs and path space measures. Those perspectives will be both of theoretical and practical value, for instance allowing to transfer methods from one to the respective other field or leading to novel algorithms for sampling from unnormalized densities. In particular, we provide a general framework by introducing a variational formulation based on divergences between path space measures of time-reversed diffusion processes. This abstract perspective can be related to the famous Schrdinger bridge problem and leads to practical losses that can be optimized by gradient-based algorithms. At the same time, it allows us to consider divergences other than the reverse Kullback-Leibler divergence that is known to suffer from mode collapse. We propose the so-called log-variance divergence, which exhibits favorable numerical properties and leads to significantly improved performance across multiple considered approaches.

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MS67

Zeroth-Order Sampling Methods for Non-Log-Concave Distributions: Alleviating Metastability

by Denoising Diffusion

We consider the problem of sampling from non-logconcave distribution, based on queries to its unnormalized density. It first describes a framework, Diffusion Monte Carlo (DMC), based on the simulation of a denoising diffusion process with its score function approximated by a generic Monte Carlo estimator. Then we provide an implementation of the oracle, based on rejection sampling. We provide convergence analyses without assuming the target distribution to be log-concave or to satisfy any isoperimetric inequality. For low dimensional distributions, ZOD-MC is a very efficient sampler, with performance exceeding latest samplers, including also-denoising-diffusion-based RDMC and RS-DMC. Last, we experimentally demonstrate the insensitivity of ZOD-MC to mode separation, discontinuity in non-convex potential, and high barriers between modes.

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MS68

UM-Bridge: User-Friendly, Scalable UQ

UM-Bridge is a flexible, language-agnostic software interface designed to integrate Uncertainty Quantification (UQ) methods with numerical models. UM-Bridge offers portability and reproducibility through containerization and provides easy access to cloud computing resources. First, I will introduce UM-Bridge itself and show how to use it to integrate cutting-edge UQ methodologies into complex numerical models. Then, I will demonstrate the application of UM-Bridge in the context of modeling the propagation of the 2011 Tohoku tsunami using shallow water equations. The primary objective is to derive precise initial displacement parameters from data collected by two buoys near the Japanese coast. To address this challenge, we introduce a fully parallelized MLMCMC method implemented in MUQ and connected to the model code via UM-Bridge.

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MS68

Multilevel Delayed Acceptance for Global Impurity Transport in Plasma-Facing Silicon Carbide

Silicon Carbide (SiC) is a promising plasma-facing material candidate for next-generation fusion devices, because of its good mechanical and thermal properties under neutron irradiation. We present a Bayesian framework for calibrating a model that predicts erosion rates of SiC impurities under well-known plasma conditions. Experimental data is provided by measurements performed in the lower diverter of the DIII-D tokamak. Because of the high computational requirements, imposed by the particle tracking code that underlies the model, we first construct an off-line surrogate, and use this surrogate in the subsequent calibration. To alleviate surrogate error in the final calibrated model predictions, we explore the use of multilevel MCMC approaches that combine samples from the surrogate with samples from the high-fidelity model.

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MS69

Derivative-Based Global Sensitivity Analysis for Models with High-Dimensional Inputs and Functional Outputs

We address global sensitivity analysis for models with high-dimensional inputs and functional outputs. We propose derivative-based global sensitivity measures (DGSMs) for such models and derive a functional DGSM-based upper bound on the generalized Sobol' indices for functional outputs. We present an efficient numerical framework for computing this upper bound by combining low-rank Karhunen-Loeve (KL) representation of the quantity of interest and adjoint-based gradient computations. Estimating the proposed DGSM-based upper bound relies on efficient gradient computation. Therefore, also addressed are models for which gradient evaluations exceed the computational budget. In this context, we present a framework for dimension reduction and surrogate modeling to accelerate uncertainty quantification. Our approach utilizes an approximation to the functional DGSMs which is motivated by ideas from active subspace methods. Moreover, we generate an efficient surrogate model by combining a truncated KL expansion of the output with polynomial chaos expansions, for the output KL modes. We demonstrate both approaches in the context of porous medium flow.

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MS69

Uncertainty Quantification in Traffic Flow Models

Vehicular traffic models as complex dynamical systems have been widely studied, however challenges for obtaining reliable forecasts are still present. Recently, it has been highlighted the dynamical system's susceptibility to uncertainties. In this talk, we will investigate how the uncertainty propagates through traffic models, affecting the output. Connections between different scales of observation will be presented in the stochastic scenario and numerical simulations will show the main results.

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MS69

Solving Parameter Dependent Eigenvalue Problems Using Taylor Series and Chebyshev Expansions

We discuss two approaches to solving the parametric (or stochastic) eigenvalue problem. One of them uses a Taylor expansion and the other a Chebyshev expansion. The parametric eigenvalue problem assumes that the matrix A depends on a parameter μ, where μ might be a random variable. Consequently, the eigenvalues and eigenvectors are also functions of μ. We compute a Taylor approximation of these functions about μ_0 by iteratively computing the Taylor coefficients. The complexity of this approach is $O(n^3)$ for all eigenpairs, if the derivatives of $A(\mu)$ at μ_0 are given. The Chebyshev expansion works similarly. We first find an initial approximation iteratively which we then refine with Newton's method. This second method is more expensive but provides a good approximation over the whole interval of the expansion instead around a single point. We present numerical experiments confirming the complexity and demonstrating that the approaches are capable of tracking eigenvalues at intersection points. Further experiments shed light on the limitations of the Taylor expansion approach with respect to the distance from the expansion point μ_0.

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MS69

Reduced Polynomial Chaos Expansion for Sensitivity Analysis in Space-Time Domain

Surrogate modeling of costly mathematical models representing physical systems is challenging since it is necessary to fulfill physical constraints in the whole design domain together with specific boundary conditions of investigated systems. Moreover, it is typically not possible to create a large experimental design due to computational burden and efficient surrogate model is thus necessary for uncertainty quantification. This contribution is focused on sensitivity analysis in recently introduced methodology for the construction of physics-informed polynomial chaos expansion (PC^2) that combines the conventional experimental design with additional constraints from the physics of the model. It is well known that a significant advantage of surrogate models in form of polynomial chaos expansions (PCE) are their possibilities in uncertainty quantification including statistical and sensitivity analysis. This feature of PCE remains also in case of PC^2 approximating partial differential equations with random parameters, despite the fact that input vector contains deterministic as well as random variables. As will be shown in this contribution, efficient sensitivity analysis can be performed during analytical post-processing of a reduced basis filtering out the influence of all deterministic space-time variables. The reduced basis can be further processed for estimation of moments, Sobol indices or for advanced distribution-based sensitivity analysis.

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MS70

A Surrogate Model-Based Bayesian Approach for Estimation Aquifer Properties in a Subsiding Basin

Land subsidence caused by groundwater over-exploitation is a geohazard with detrimental effects on structures and aquifer capacity. Advances in monitoring techniques, especially the Interferometric Synthetic Aperture Radar (InSAR) technique, allow in principle to characterize the aquifer properties by Bayesian inversion. However, the associated finite element (FE) models are usually too expensive for Markov Chain Monte Carlo (MCMC) algorithms. To address this issue, we use a sparse grid collocation method to approximate the FE solutions, by interpolating the results on a handful of well-selected parameter locations, and propose a procedure to characterize the aquifer properties in a subsiding basin using piezometric records and InSAR-based displacement measurements. The approach is applied to calibrate the hydraulic conductivity and compressibility of the Alto Guadalentn Valley aquifer system in Spain. Hydraulic conductivity is first calibrated against a long-time series of piezometric records, and in a second step the compressibility is calibrated against InSAR data to guarantee the fulfillment of the coupled groundwater flow and mechanical FE model. It is found that the applied coupled model can properly capture the aquifer system responses to groundwater withdrawal, and the sparse grid can approximate the numerical solutions efficiently and accurately. Furthermore, this strategy can significantly reduce the uncertainty of parameters of interest.

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MS70

Learning Deep: Probabilistic Forward and Inverse Methods in Large-Scale Geological Models

The analysis focuses on the information value provided by a probabilistic approach in geological modelling and characterization. We will focus on Stratigraphic forward models (SFMs), that are typically used to obtain model-based predictions of the architecture of sedimentary bodies. To this end simulations typically encompass large spatial and temporal scales, i.e. domain dimensions of ≈ 100 km and accumulation time of millions of years. SFMs are process-based tools that require hundreds of input parameters tied to individual processes, encompassing sediment transport, carbonates build-up, sea level variations, hydrodynamic and sediment source characteristics. These inputs are usually affected by uncertainty. We will show the application of a suite of uncertainty quantification and stochastic model calibration algorithms for the characterization of sedimentary successions in large scale systems. Our work combines sensitivity analysis, model reduction techniques and particle swarm optimization algorithms. Results obtained in real test cases are postprocessed to assess (i) the uncertainty and practical identifiability of model parameters given a set of observations, (ii) spatial distribution of lithologies to be employed in assessing potential subsurface fluid extraction or storage.

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MS70

Quantification of Uncertainties in Simulation of Wall-Bounded Turbulent Flows

Scale-resolving approaches such as direct numerical simulation (DNS) and large eddy simulation (LES) result in the spatio-temporal fields for turbulent flows, and hence are capable of revealing the flow physics. Two main challenges to deal with, when using these approaches, are the high computational cost particularly at high Reynolds numbers relevant to engineering applications, and accurately accounting for the uncertainties from different sources. We present our recent progress on quantifying uncertainties in the quantities of interest (QoIs) of LES and DNS of wall-bounded turbulent flows. First, we address the influence of the numerical/computational parameters such as grid resolutions and filtering on the the accuracy of the QoIs using non-intrusive polynomial chaos expansion and Sobol sensitivity indices. To this end, two open-source computational fluid dynamics (CFD) software are investigated. Then, the accurate estimation of uncertainty in turbulence statistics due to the finite time-averaging will be thoroughly discussed. Finally, we introduce a variation of the Gaussian process regression that allows for combining uncertainties from the parametric and finite time-averaging sources. The resulting framework can be useful for uncertainty quantification of turbulent flow simulations, systematic comparison between the CFD software, and drawing best-practice guidelines to achieve accurate simulations.

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MS70

Stabilised Dynamical Low-Rank Methods for Random Advection-Dominated Problems

The efficient and accurate simulation of random unsteady advection-dominated problems in a multi-query context is challenging. On the one hand, those problems are not amenable to the POD paradigm. While the solution may exhibit a low-rank structure at all times, the subspaces capturing that structure can vary significantly over time. The Dynamical Low Rank framework can be an interesting alternative: the random field $u(t, x, \xi)$ is approximated by an expansion $\sum_{i=1}^{R} U_i(t, x)Y_i(t, \xi)$, where the physical (U_i) and stochastic (Y_i) modes evolve in time, yielding a quasi-optimal approximation of the best rank-R approximation. On the other hand, the use of the standard Finite Element method is also problematic as the numerical solutions thus obtained display oscillations. These numerical artifacts are unphysical and must be removed or at least alleviated. To tackle this, we introduce a framework of stabilised Dynamical Low Rank methods. The framework naturally integrates any stabilisation technique that is expressed as a generalised Petrov-Galerkin method for a time-dependent problem. The streamline Upwind/Petrov-Galerkin and Interior Penalty methods fall into this category. A family of time-stepping algorithms is introduced and their properties analysed. Under certain assumptions, the stabilised DLR method is shown to inherit the properties of the stabilised full-order model. Numerical experiments will illustrate the effectiveness of the stabilising methods.

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MS71

CUQIpy: Computational Uncertainty Quantification for Inverse Problems in Python

In this talk we present CUQIpy (pronounced cookie pie) - a new computational modelling environment in Python that uses uncertainty quantification (UQ) to access and quantify the uncertainties in solutions to inverse problems. The overall goal of the software package is to allow both expert and non-expert (without deep knowledge of statistics and UQ) users to perform UQ related analysis of their inverse problem while focusing on the modelling aspects. To achieve this goal the package utilizes state-of-the-art tools and methods in statistics and scientific computing specifically tuned to the ill-posed and often large-scale nature of inverse problems to make UQ feasible. We showcase the software on problems relevant to imaging science such as computed tomography and partial differential equation-based inverse problems. CUQIpy is developed as part of the CUQI project at the Technical University of Denmark and is available at https://github.com/CUQI-

DTU/CUQIpy.

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MS71

CLAIRE: Scalable Algorithms for Diffeomorphic Image Registration

We discuss numerical methods for optimal control problems governed by geodesic flows of diffeomorphisms. Our contributions are designing effective numerical methods and fast computational kernels that scale on heterogeneous, high-performance computing platforms. We discuss efficient numerical methods, implementation aspects, and performance of the proposed method for inference and UQ. The considered inverse problem is infinite-dimensional in principle. We seek to establish spatial correspondences between two views (images) of the same object. In principle, these correspondences are modeled as geodesic flows of diffeomorphisms. The solution of the associated optimality conditions poses significant mathematical and numerical challenges; the optimization problem is non-convex and non-linear, which, upon discretization, results in high-dimensional ill-conditioned systems. Our solvers are based on state-of-the-art algorithms to enable fast convergence and short runtime. We use adjoint-based first- and second-order methods for numerical optimization. We report results for real and synthetic data to study the rate of convergence, time-to-solution, numerical accuracy, and scalability of our solvers. As a highlight, we will showcase results for a GPU-accelerated implementation termed CLAIRE that allows us to solve clinically relevant 3D image registration problems with high accuracy in under 5 seconds on a single GPU and scales up to 100s of GPUs.

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MS71

UM-Bridge: Enabling Advanced UQ from Prototype to Supercomputer

UM-Bridge is a universal software interface for linking virtually any UQ method to any numerical simulation model. It further allows straightforward scaling of UQ from prototypes to large-scale applications on HPC and cloud clusters. UM-Bridge currently supports C++, Python, Matlab, R and Julia, and seamless integrations exist for a number of UQ packages. We thereby bridge the gap between advanced UQ and state-of-the-art numerical simulation, and lower the entry barrier to UQ for a wide audience. In addition, based on that technology, we are developing the first library of ready-to-run UQ benchmark problems as a community-driven project. This talk gives some background on UM-Bridge, introduces the benchmark library and shows applications pairing recent UQ methods with challenging numerical models on large clusters.

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MS71

MParT: Scaling Measure Transport for High-dimensional Conditional Inference Problems

MParT (Monotone Parameterization Toolkit) is an open-source C++ toolkit for constructing deterministic transport maps, with bindings to Python, Julia, and MATLAB. Transportation of measure has shown immense power as an emerging method for probabilistic inference, density estimation, and generative modeling. However, many tools to perform it suffer from intractability when applied to large sample sizes or high-dimensional problems. In this talk, we present novel methods that work on the interface between scalable software and tractable algorithm development. In particular, we show that clever parameterizations of transport maps in MParT are necessary for both efficient computation and sufficient expressivity. Further, we show how building the function class for the map reflects knowledge of our parameters of interest and their relationships. Finally, we use transport to hybridize modern methods for reducing the dimension of the system and more traditional methods (such as quadrature), which effectively compute quantities of interest but might be only tractable for well-understood, low-dimensional distributions.

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MS72

Ethical Decision Support using Digital Twins in climate change applications

Environmental simulations, which are driven under unknown future climate, underpin digital twin models that are then used as decision support tools. Subsequent decisions are therefore conditioned on these climate scenarios, thus introducing uncertainty in regard to the ways in which these scenarios are believed to be informative on reality. We present foundationally principled model synthesis aimed at quantifying uncertainty over such modelling judgements. Work such as this is an ethical imperative in the age of AI and machine learning, whereby it is the responsibility of modellers to acknowledge and communicate such uncertainties to users when providing decision support through the use of complex systems.

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MS72

Linked Deep Gaussian Process Emulation

Modern scientific problems often span multiple disciplines, necessitating the integration of distinct computer models, each with unique functional complexities, computation times, and programming environments. In this talk, we first review the Gaussian process (GP) emulation, and then introduce its advancements to linked Gaussian process (LGP) and deep Gaussian process (DGP) emulations that offer powerful tools to address emulation challenges related to computer model networks and computer models with non-stationary behaviours. We subsequently present the linked deep Gaussian process (LDGP) emulation, that conceptualises a computer model network as a DGP with partial exposure of its hidden layers. We develop a method for inferring these partially exposed deep networks, where each model in the network can be independently and automatically emulated using a (D)GP surrogate and then linked together. Using both synthetic and empirical examples, implemented by our freely available R package dgpsi on CRAN, we demonstrate that our DGP and LDGP emulators, enhanced by sequential designs and automatic structure selection, deliver significantly better performance than conventional GP emulators in terms of predictive accuracy, uncertainty quantification, and computation.

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MS72

Digital Twinning for Risk Assessment for Natural Hazards

Wildfire is a catalyst for landcover change that can substantially increase the potential for devastating and destructive debris flow hazards. Debris flows, or fast-moving landslides that consist of a mixture of water, mud, and rock, initiate after fires when surface water runoff rapidly erodes sediment on steep slopes. Numerical models of post-fire debris flow bulking and runout are computationally intensive. These models depend on poorly constrained and difficult to measure parameters related to fire-altered soil and vegetation, some of which change in time. Further, the development of debris flows (as opposed to clear flows) also depends on the rainfall intensity of potential storms. To date, modeling-based hazard analysis has focused on if' a debris flow might be triggered on a given fire scared hillside, and not on the extent or footprint of potential debris flow runouts. We employ Gaussian process emulators to high-dimensional debris flow model output to quantify uncertainties and aid in model-based hazard assessments of post-fire debris flow inundation.

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MS73

Coordinating High-Dimensional Sparsification with Projective Integral Updates

It is often quite challenging to efficiently train learning models with high dimensionality, such as neural networks. Choices among optimization procedures, regularization strategies, and hyperparameter searches can significantly impact the final quality of predictions. This is because limited computational resources will always impede comprehensive exploration of high-dimensional posteriors. Thus, the trajectory of optimization is at least as important as how we incorporate model uncertainty into predictions. In order to obtain models with well-coordinated sparsity and strong predictive performance, we need economical heuristics that support skillful navigation. Projective integral updates allow us to quickly approximate the shape of the local loss topography (the negative log posterior) using standard backpropagation. We examine how this structural information supports efficient sparsification decisions during training.

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MS73

On Prior Specification in Bayesian Neural Networks and Gaussian Processes

Bayesian methods promise to augment accurate predictions provided by modern neural networks with well-calibrated predictive uncertainties. Despite their promise, Bayesian approaches to neural networks struggle with both, producing useful uncertainties and accurate predictions. The high-dimensional space spanned by neural network weights makes specifying meaningful priors and inferring the resulting posterior distribution challenging! In this talk, I will first describe our work on side-stepping the high-dimensionality of the problem by using continuous shrinkage priors that aggressively shrink a subset of the network's weights to zero and show that they provide better-calibrated uncertainties and predictions than Gaussian priors when used with variational inference. Next, focusing more broadly on the issue of prior specification, I will restrict myself to the simpler setting of Gaussian processes (GP) and describe our recent work on probing the robustness of GPs to the choice of the prior kernel and describe how the resulting method provides a model criticism tool for practitioners to flag robustness issues in their GP-based analysis.

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MS73

Understanding Uncertainty-Based Active Learning

Uncertainty-based Active Learning (UAL) operates by querying the label(s) of the selected pivotal samples from an unlabeled dataset based on prediction uncertainty so that the labeling cost can be minimized for model training. The efficacy of UAL depends on the model capacity as well as the adopted uncertainty-based acquisition function. Within the context of this study, our analytical focus is directed towards understanding how the machine learning model capacity may affect UAL efficacy. Through comprehensive theoretical analysis and simulation studies, we conclusively demonstrate why UAL may not always perform better than typical random sampling based model training, especially when the underlying ground truth does not lie in the machine learning model class.

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MS73

Hyper-Parameters Estimation in Bayesian Models

Hyper-parameters play a crucial role in shaping the behavior of Bayesian models and can have a significant impact on their performance and generalization ability. Bayesian models can have a high number of hyper-parameters, particularly in complex models like hierarchical Bayesian models or deep probabilistic models. Managing and tuning a large number of hyper-parameters can be computationally intensive and require careful attention. We will propose an efficient numerical algorithm of hyper-parameters estimation in sparse Bayesian learning models and present its comparisons with other popular methods of hyper-parameters estimation.

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MS74

A Machine Learning Framework to Correct under-Resolved Climate Simulations Using Nudged Data Sets

Due to the rapidly changing climate, the frequency and severity of extreme weather, such as storms and heatwaves is expected to increase drastically over the coming decades. Accurately quantifying the risk of such events with high spatial resolution is a critical step in the implementation of strategies to prepare for and mitigate the damages. As fully resolved simulations remain computationally out of reach, policy makers must rely on coarse resolution climate models which either parameterize or completely ignore subgrid scale dynamics. In this work we propose a machine learning framework to debias under-resolved simulations of complex and chaotic dynamical systems such as atmospheric dynamics. The proposed strategy uses "nudged' simulations of the coarse model to generate training data designed to minimize the effects of chaotic divergence. We illustrate through a prototype QG model that the proposed approach allow us to machine learn a map from the chaotic attractor of under-resolved dynamics to that of the fully resolved system. In this way we are able to recover extreme event statistics using a very small training dataset.

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MS74

Lagrangian Uncertainty Quantification and Information Inequalities in Stochastic Flows

We develop a systematic information-theoretic framework for quantification and mitigation of error in probabilistic path-based (Lagrangian) predictions which are obtained from dynamical systems generated by uncertain (Eulerian) vector fields. This work is motivated by the desire to improve Lagrangian predictions in complex dynamical systems based either on analytically simplified or data-driven models. We derive a hierarchy of general information bounds on the uncertainty in estimates of statistical observables $E^{\nu}[f]$, evaluated on trajectories of the approximating dynamical system, relative to the true observables $E^{\mu}[f]$ in terms of certain φ-divergencies $D(\mu||\nu)$ which quantify discrepancies between probability measures μ associated with the original dynamics and their approximations ν. We then derive bounds on $D(\mu||\nu)$ itself in terms of the Eulerian fields. This framework provides a rigorous way for quantifying and mitigating uncertainty in Lagrangian predictions due to Eulerian model error. Links to uncertainty quantification in Data Assimilation techniques will also be mentioned.

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MS74

Derivative-Free Loss Method for Homogenization

We propose a neural network-based approach to the homogenization of multiscale problems. The proposed method uses a derivative-free formulation of a training loss, which incorporates Brownian walkers to find the macroscopic description of a multiscale PDE solution. Compared with other network-based approaches for multiscale problems, the proposed method is free from the design of handcrafted neural network architecture and the cell problem to calculate the homogenization coefficient. The exploration neighborhood of the Brownian walkers affects the overall learning trajectory. We determine the bounds of micro- and macro-time steps that capture the local heterogeneous and global homogeneous solution behaviors, respectively, through a neural network. The bounds imply that the computational cost of the proposed method is independent of the microscale periodic structure for the standard periodic problems. We validate the efficiency and robustness of the proposed method through a suite of linear and nonlinear multiscale problems with periodic and random field

coefficients.

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MS74

Discretization-Invariant Extension and Algorithms of Operator Learning on Solving Heterogeneous Multiscale PDE Problems

In this presentation, we will delve into the topic of invariant extensions in operator learning. The concept of discretization-invariant neural operators is pivotal, as it allows for the disparate discretization of various input functions. This attribute holds significant relevance, particularly in scenarios involving heterogeneous datasets with multiscale and multifrequency characteristics. First, we will explore theoretical extensions to the widely adopted deep operator neural network (DON). This extension, referred to as Basis Enhanced Learning (Bel), ensures invariance to input function discretization, addressing an essential need in the field. Additionally, we will introduce a novel training methodology inspired by federated learning. This approach not only diminishes the reliance on input function discretization but also enhances the overall efficiency and accuracy of the method.

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MS75

Solving PDE-Based Bayesian Inverse Problems Using CUQIpy

Inverse problems, particularly those governed by Partial Differential Equations (PDEs), are prevalent in various scientific and engineering applications, and uncertainty quantification (UQ) of solutions to these problems is essential for informed decision-making. In this talk, we present how CUQIpy, a Python software package for computational UQ in inverse problems using a Bayesian framework, is extended to solve PDE-based Bayesian inverse problems. We devise a general framework that allows the integration of PDEs in CUQIpy, whether expressed natively or using third-party libraries such as FEniCS. CUQIpy offers concise syntax that closely matches mathematical expressions, streamlining the modeling process and enhancing the user experience. The versatility and applicability of CUQIpy to PDE-based Bayesian inverse problems are demonstrated in examples covering parabolic, elliptic, and hyperbolic PDEs. This includes problems involving the heat and Poisson equations and application case studies in electrical impedance tomography (EIT) and photo-acoustic tomography (PAT). We additionally present a case study for brain efflux using real data. These examples showcase the softwares efficiency, consistency, and intuitive interface. Our comprehensive approach to UQ in PDE-based inverse problems provides accessibility for non-experts and advanced features for experts.

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MS75

Ensemble-Based Accelerated Uncertainty Quantification for Climate Model Forecasting

Process-based climate models are a collection of partial differential equations that must represent dynamics across many spatial and temporal scales. It is infeasible to resolve all of these scales. Instead, the physics at the smallest scales is represented by empirical or data-driven parameterization schemes that link what is unresolvable to variables resolved on the grid scale. A large source of uncertainty in climate predictions comes from the calibration of parameters in such parameterization schemes, and these uncertainties are generally not quantified. Despite a wealth of observation data, satellites, field campaigns, targeted high-resolution simulation, uncertainties are not quantified in practice due to the large computational expense of running PDE models. In this talk we will demonstrate our successful approach to learn a suitable parameter distribution from statistical data. Our method, Calibrate-Emulate-Sample (CES), combines ensemble Kalman processes, machine learning, and statistical sampling tools applied in a black-box fashion to obtain approximate posterior distributions. CES smooths and accelerates the inversion, requiring 1000s of times fewer model evaluations than classical approaches. Time permitting, we shall explore some successes of this approach in Atmosphere, Ocean, and Land components of a climate model being developed at the Climate Modelling Alliance.

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MS75

Kernel Approaches to Ensemble Kalman Filters and Sequential Monte Carlo

In this talk, we will discuss possible approaches how kernel embeddings can improve the performance of certain methodologies for filtering and other inverse problems. One important substep that we will focus on is the kernel mean outbedding.

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MS75

Non-Parametric Bayesian Inference for Diffusion Processes

A wide range of systems in science, engineering and economics can be modeled by stochastic processes, or more precisely diffusion processes. Data of such processes is often available in the form of stochastic trajectories or statistics like expectation values or probability distributions. On the other hand, the underlying dynamics in the form of the drift and diffusion functions are frequently unknown. We discuss a procedure for the inference of drift and diffusion functions from trajectory data in a Bayesian framework. We pose the problem in a function space setting, and utilize the duality of diffusion processes with their generators, i.e. PDE operators. These generators allow us to derive PDE-based forward models from the Kolmogorov equations. For the evaluation of statistics from the posterior, we firstly discuss an optimization-based approach via the Laplace approximation. In particular, we elaborate on the underlying algorithms, which make use of the low-rank properties of the parameter-to-observable mapping. This low-rank structure allows for numerical procedures that converge independently of the chosen discretization of the formally infinite-dimensional problem. As a second approach, we introduce dimension-independent Markov Chain Monte Carlo methods. These methods can be further enhanced through incorporation of the Laplace approximation, resulting in a significant reduction in mixing times. We finally show some examples to demonstrate the presented methods.

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MS76

Hyper-Differential Sensitivity Analysis to Support Calibration of Ice Sheet Models

Understanding ice sheet melting is critical for analyzing the climate system and its response to increasing global temperatures. Models for ice sheets involve complex large-scale partial differential equations which depend on unobservable quantities corresponding to processes on the interior and bottom of the ice sheet. Hence, calibration of the ice sheet models to estimate such quantities is crucial to enable accurate predictions. However, such calibration is challenging due to the dimension of the uncertain parameters and the computational complexity of the model. In this talk, we present hyper-differential sensitivity analysis as a computational tool which complements numerical optimization to enhance the calibration of ice sheet models. We introduce the mathematical foundations of the proposed approach and demonstrate it on a model for the Greenland ice sheet.

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MS76

Decision Making / Data Assimilation on Complex Networks Affected by Weather Extremes

Resilience of critical infrastructure has become a major socio-economic challenge. We specifically address the decision structure that a community follows in restoring the infrastructure to operating conditions, as economically expedient as is possible, after the system is hit by climactic stresses. In this talk we outline two methodologies for creating a decision process. One of these produces a decision process for restoration that exchanges optimality for robustness. The other could be used by stakeholders to assess the effectiveness of different policies.

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MS76

Physics-Based and Data-Driven Modeling and Data Assimilation for Wildfire Smoke in the Stratosphere

The quantitative assessment of wildfire dynamics encounters challenges due to computational expenses associated with conducting extensive large-scale atmospheric simulations and managing high-dimensional spatio-temporal outputs. In this work, we present a probabilistic framework for predicting atmospheric transport of wildfire smoke in the stratosphere using a limited number of atmospheric simulations. Various uncertainty quantification and machine learning methods (e.g., polynomial chaos expansion, probabilistic learning on manifolds, and normalizing flows) are applied upon the simulation data of the 2020 British Columbia case for comparison. The joint density function between the model inputs and outputs are built. Moreover,

this statistical dependency allows for calibrating the distribution of inputs based on the satellite observation. An illustrative study integrating a hundred simulations by the Energy Exascale Earth System Model (E3SM) and satellite observation is investigated to demonstrate the presented approach.

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MS76

Deep Learning-Based Data Assimilation and Uncertainty Quantification with Generative Priors and Multimodal Sensing Data in Subsurface Systems

Subsurface carbon storage has a large potential to reduce greenhouse gas emission. With traditional approaches high computational expenses for large-scale problems often hinder us to perform rigorous climate and subsurface modeling resulting in less accurate prediction with high uncertainty. To overcome this limit, we develop and apply deep learning (DL)-based forward and inverse modeling framework to accelerate forecasting through real-time updates of model parameters with uncertainty quantification (UQ). For DL-based surrogate models of pressure and fluid saturation in heterogeneous property fields, modified DeepONet architecture and convolutional neural networks-long-short term memory are used. For data assimilation, the latent space much smaller than the physical parameter space is updated with multi-modal observation data. The updated latent space is fed to a deep generative prior(s) (e.g., conditional variational autoencoder, diffusion model) for generating physical parameter fields as input to DL-based forward surrogate models to predict pressure and multiphase saturation. Additionally, posterior covariance analysis in the latent space provides an ensemble generation of parameters for rigorous UQ. We will highlight the efficiency and robustness of proposed methods for real-time forecasting and applicability using a real field demonstration project of geologic carbon storage. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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MS77

Probabilistic Neural Operators

In scientific machine learning, neural operators have introduced a new frontier over the past few years. However, conventional neural operators are often deterministic and do not account for uncertainty due to noisy and limited data. In this work, we discuss two algorithms for developing probabilistic neural operators. The first algorithm is inspired from the contemporary reinforcement learning framework and uses randomized prior network to develop a probabilistic neural operator. The second variant is more principled and explores the possibility of combining Gaussian process and neural operator. We illustrate the performance of the two algorithms in developing probabilistic wavelet neural operator. The performance of the probabilistic wavelet neural operator is illustrated on several benchmark examples from computational mechanics.

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MS77

Error Bounds and Rates for Fourier Neural Operators

Fourier Neural Operators (FNO) are a class of General Neural Operators that take advantage of the fast Fourier transform to parameterize infinite-dimensional operators in Fourier space using a finite number of parameters. One advantage of this architecture is its discretization-invariance; a model trained at one discretization can be used at a different discretization without significant loss of accuracy. However, prior work has ignored the error that results from performing a convolution on a grid. In this talk, we discuss the error that results from this necessary approximation and its impact on the usefulness of FNO.

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MS77

PDE-Constrained Gaussian Process Surrogate Modelling with Uncertain Data Locations

Gaussian process regression is widely applied in computational science and engineering for supervised learning owning to its kernel-based and probabilistic nature. In this work, we propose a Bayesian approach that integrates the variability of input data into Gaussian process regression to learn function approximation and linear partial differential equations. Considering two types of observables – noise-corrupted outputs with fixed inputs and those with prior-distribution-defined uncertain inputs, a posterior dis-

tribution is estimated via a Bayesian framework to infer the uncertain data locations. Thereafter, such quantified uncertainties of inputs are incorporated into Gaussian process predictions by means of marginalization. The setting of two types of data aligned with common scenarios of learning partial differential equations, where the data of boundary conditions, initial condition and governing equations are known exactly and measured data of solution may involve uncertainties. The effectiveness of this new regression technique is demonstrated through several numerical examples, in which a consistently good performance of generalization is observed, while a substantial reduction in the predictive uncertainties is achieved by the Bayesian inference of uncertain inputs.

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MS77

Measuring Uncertainties over Sets of Operators Consistent with Observed Actions

The data-consistent approach to stochastic inverse problems has recently been adapted to solve ill-posed parameter identification inverse problems. Similar to a Bayesian approach, an initial or prior density is proposed for the parameter of interest. However, rather than utilizing the data-likelihood distribution, the initial density is updated using the ratio of observed and predicted distributions of a sufficient statistic derived from the data-likelihood. The resulting maximum updated density point (MUD) point has been shown to have less bias compared to traditional Bayesian maximum a posteriori (MAP) points. In our current research, we analyze the consequences of utilizing the data-consistent approach in the context of operator learning. We analyze the bias and variance of the MUD operator and discuss the potential benefits and drawbacks of estimating the uncertainty associated with operator learning in a data-consistent framework.

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MS78

Why One Single Surrogate Model Cannot Be Used for All Applications

In this presentation, we explore the pivotal question of whether a universal surrogate model can effectively meet the diverse requirements of various applications in computational modeling. Our investigation spans diverse domains, uncovering inherent challenges stemming from the distinct characteristics of each application. The discussion underscores the significance of tailoring surrogate models to specific contexts, taking into account factors such as computational cost for training, size of the training data, input parameter space, characteristics of state space, model complexity, and unique application demands. Through insightful case studies and pragmatic considerations, this talk seeks to provide guidance for researchers and practitioners navigating the intricacies of surrogate modeling, aiming for optimal performance across a broad spectrum of applications.

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MS78

Surrogate-Enabled Inference of High-Dimensional Systems Through Dimension Reduction: Applications to Fluid Plasma Simulations

Fluid models of plasma offer the ability to characterize complex plasma phenomena in a manner computationally accessible to practical engineering applications, such as design optimization and risk analysis. However, fluid plasma models require ad hoc closures to inherently kinetic effects in the underlying plasma behavior. These kinetic effects are better resolved by particle-in-cell (PIC) plasma simulations, but such codes are computationally intensive on time and length scales of interest. While PIC simulations cannot be used directly for design optimization due to expense, they are a valuable source for studying plasma instabilities and informing fluid closure models. To this end, we apply adaptive surrogate methods based on sparse grids to approximate the outputs of a PIC code over a set of design variables. We additionally consider the approximation of high-dimensional spatiotemporal outputs, such as field quantities and distribution functions, by way of dimension-reduction techniques. We study the challenges of effectively building a surrogate for noisy PIC outputs and of balancing surrogate prediction error in the latent space with reconstruction error. Time-permitting, we also apply the surrogate to an outer-loop inference of PIC calibration parameters.

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MS78

Hypernetwork-Based Meta-Learning for Low-Rank Physics-Informed Neural Networks

In various engineering and applied science applications, repetitive numerical simulations of partial differential equations (PDEs) for varying input parameters are often required (e.g., aircraft shape optimization over many design parameters) and solvers are required to perform rapid execution. In this study, we suggest a path that potentially opens up a possibility for physics-informed neural networks (PINNs), emerging deep-learning-based solvers, to be considered as one such solver. Although PINNs have pioneered a proper integration of deep-learning and scientific computing, they require repetitive time-consuming training of neural networks, which is not suitable for many-query scenarios. To address this issue, we propose lightweight low-rank PINNs containing only hundreds of model parameters and an associated hypernetwork-based meta-learning algorithm, which allow efficient solution approximations for varying PDE input parameters. Moreover, we show that the proposed method is effective in overcoming a challenging issue, known as "failure modes" of PINNs.

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MS78

Bayesian Calibration of Stochastic Agent Based Model via PCA Based Surrogate Modeling

Calibrating stochastic models requires addressing the usual model form, measurement, and sampling errors, but also requires accounting for errors in the instantiation of model simulations. This additional error can be addressed with increased sampling, but Agent Based Models (ABMs) are usually prohibitively expensive, limiting the number of feasible runs. ABMs also typically involve discrete interactions which restricts the usage of smooth surrogates and derivative-accelerated samplers. In this presentation, we outline a straightforward and fast surrogate technique which relies on a PCA decomposition of the ABM outputs over time in combination with a random forest mapping from ABM parameters to PCA weights. This approach allows for dramatic acceleration in ABM sampling while still capturing discrete and nonlinear model dynamics. We demonstrate these surrogates use for calibration with adaptive MCMC for both the mean ABM outputs and for outputs from individual ABM instantiations. Finally, the results of these varied stochastic calibration approaches are analyzed and compared.

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MS79

Hierarchical Emulation of Stochastic Agent-Based Models

Agent-based models are common in determining prevalence, spread, inherent characteristics of a disease; their complexity, high-dimensional parameter space, and stochasticity can complicate the process of inference and prediction. A hierarchical approach to emulation, where both the simulator response and stochasticity are emulated and linked, can alleviate the above complications when coupled to a process of history matching. I will motivate this approach in the context of modelling human papillomavirus (HPV) via HPVsim, using Bayes linear covariance emulation. The non-implausible space obtained can be used for predictions about future trends of the disease, and the efficacy of possible interventions - I discuss means by which emulation can most optimally be used to frame policy decisions and posterior analysis via novel stopping conditions on history matching. For computationally expensive agent-based models, such considerations speed the process of calibration while allowing robust inference, and aid in experimental design for future information-gathering campaigns.

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MS79

Bayes Linear Emulation with Uncertain Inputs

Emulators typically capture uncertainties in our knowledge of simulator behaviour, which themselves seek to reflect the behaviour of corresponding real-world processes, at points in the input space for which the simulator has not been run due to computational intensity issues. However, it is less common for this uncertainty specification to capture uncertainty surrounding the values of the inputs to the model, which are often assumed known. We develop general modelling methodology with uncertain inputs in the context of the Bayes linear paradigm, which involves adjustment of second-order belief specifications over all quantities of interest only, without the requirement for probabilistic specifications. We demonstrate our emulation methodology on a motivating epidemiological simulator chain to model the impact of an airborne infectious disease.

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MS79

Adaptive Design of Experiments with Gaussian Processes: Single and Multi-Level Case

Gaussian process (GP) emulators are generally regarded as the gold standard surrogate model for approximating complex computer models. Traditionally, GPs are constructed based on a set of design points that are selected at once in a space-filling manner. Recently though there has been a lot of interest in adaptive designs where the choice of the next sample depends on the previously observed model outputs. We address this problem by proposing a novel adaptive design criterion called VIGF (variance of improvement for global fit). The method is extended to the multi-fidelity case where the expensive high fidelity model is predicted with the assistance of a lower fidelity computer code. This is performed via hierarchical kriging. The applicability of our method is assessed on a bunch of test functions and its performance is compared with several sampling strategies. The results suggest that our method has a superior performance in predicting the benchmark functions in most cases.

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MS79

Statistically Approximating a High Resolution Flood Model

In the U.S. there have been at least ten $1 billion riverine floods each year from 2015 to 2022. We can learn about riverine flooding to better inform policy with physics-based flood models. Previous research has found that calibrated high resolution flood projections tend to be more realistic for spatially heterogeneous areas like cities. However, calibrating a flood hazard model using projections at the desired high resolution may be computationally infeasible. Previous attempts at efficient methods to approximate high resolution projections neglect uncertainty in their interpo-

lations due to the impact of increasing spatial resolution. We propose a physics-informed hierarchical model that accounts for this previously neglected uncertainty source. Our model approximates the high resolution flood projection for any location using (1) lower resolution flood projections over the same spatial domain and (2) a high resolution digital elevation model. Our approach boasts improved uncertainty quantification compared to previous approaches

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MS80

Distributional Uncertainty Propagation via Optimal Transport

In this talk I will challenge the standard uncertainty models, e.g., robust (norm-bounded) and stochastic (one fixed distribution, e.g., Gaussian), and propose to model uncertainty via Optimal Transport (OT) ambiguity sets. These constitute a very rich uncertainty model, which enjoys many desirable geometrical, statistical, and computational properties, and which: (1) naturally generalizes both robust and stochastic models, and (2) captures many additional real-world uncertainty phenomena (e.g., black swan events). I will then show that OT ambiguity sets are analytically tractable: they propagate easily and intuitively through linear and nonlinear (possibly corrupted by noise) transformations, and the result of the propagation is again an OT ambiguity set or can be tightly upper bounded by one. In the context of dynamical systems, this allows to consider multiple sources of uncertainty (e.g., initial condition, additive noise, multiplicative noise) and to capture in closed-form, via an OT ambiguity set, the resulting uncertainty in the state at any future time. The resulting OT ambiguity sets are also computationally tractable, and can be directly employed in various distributionally robust control formulations that can optimally trade between safety and performance.

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MS80

Sliced-Wasserstein Distances and Flows on Hadamard Manifolds

While many Machine Learning methods were developed or transposed on Riemannian manifolds to tackle data with known non Euclidean geometry, Optimal Transport (OT) methods on such spaces have not received much attention. The main OT tool on these spaces is the Wasserstein distance which suffers from a heavy computational burden. On Euclidean spaces, a popular alternative is the Sliced-Wasserstein distance, which leverages a closed-form solution of the Wasserstein distance in one dimension, but which is not readily available on manifolds. In this work, we derive general constructions of Sliced-Wasserstein distances on Hadamard manifolds: Riemannian manifolds with non-positive curvature which include among others hyperbolic spaces or the space of symmetric positive definite matrices. Additionally, we derive non-parametric schemes to minimize these new distances by approximating their Wasserstein gradient flows.

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MS80

Wasserstein Mirror Gradient Flow as the Limit of the Sinkhorn Algorithm

In this talk, we study the sequence of marginals obtained from iterations of the Sinkhorn or IPFP algorithm and show that under a suitable time and regularization scaling, the marginals converge to an absolutely continuous curve on the Wasserstein space. This limit, which we call the Sinkhorn flow, is an example of a Wasserstein mirror gradient flow, a concept we introduce here inspired by the well-known Euclidean mirror gradient flows. In the case of Sinkhorn, the gradient is that of the relative entropy functional with respect to one of the marginals and the mirror is half of the squared Wasserstein distance functional from the other marginal. Interestingly, the norm of the velocity field of this flow can be interpreted as the metric derivative with respect to the linearized optimal transport (LOT) distance. We provide examples to show that these flows can have faster convergence rates than usual gradient flows. We also construct a Mckean-Vlasov SDE whose marginal distributions give rise to the same flow.

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MS80

Scalable Unbalanced Optimal Transport by Slicing

Optimal transport (OT) has emerged as a powerful framework to compare probability measures, a fundamental task in many statistical and machine learning problems. Substantial advances have been made over the last decade in designing OT variants which are either computationally and statistically more efficient, or more robust to the measures and datasets to compare. Among them, sliced OT distances have been extensively used to mitigate optimal transport's cubic algorithmic complexity and curse of dimensionality. In parallel, unbalanced OT was designed to allow comparisons of more general positive measures, while being more robust to outliers. In this paper, we propose to combine these two concepts, namely slicing and unbalanced OT, to develop a general framework for efficiently comparing positive measures. We propose two new loss functions based on the idea of slicing unbalanced OT, and study their induced topology and statistical properties. We then develop a fast Frank-Wolfe-type algorithm to compute these loss functions, and show that the resulting methodology is modular as it encompasses and extends prior related work. We finally conduct an empirical analysis of our loss functions and methodology on both synthetic and real datasets, to illustrate their relevance and applicability. This is a joint work with Thibault Sjourné, Clément Bonet, Kilian Fatras, and Nicolas Courty. The corresponding paper is https://arxiv.org/abs/2306.07176

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MS81

Uncertainty Quantification of Sampled Neural Net-

works

Neural networks are widely used for solving problems in various domains. However, their training procedure is often computationally costly, while their predictions are difficult to analyze. The introduction of sampled networks and the efficient SWIM algorithm [Bolager et al., Sampling weights of deep neural networks, 2023] opened the way for both theoretical and practical analysis of neural networks. The presented work uses this opportunity to formulate a Bayesian view of sampled networks. As these networks allow fast uncertainty evaluation, we first investigate the finite-width case. Similarly to classical neural networks, we also consider the infinite-width limit and show the correspondence between sampled networks and Gaussian processes. Additionally, we provide theoretical bounds on the out-of-domain behavior of these networks and support the findings with experimental results.

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MS81

Entropy Stable Model Reduction of Hyperbolic Systems on Nonlinear Manifolds

Model reduction of hyperbolic systems is a difficult topic. This is a result of the fact that solutions of such systems typically do not evolve in low-dimensional linear subspaces. This elides the use of well-established linear model reduction techniques. To solve these problems we describe how we can construct novel reduced order models (ROMs) of hyperbolic systems on spaces parameterized by nonlinear functions. The ROMs are constructed such that important convex entropy functionals are adequately conserved or dissipated depending on the discrete solution's regularity, a concept referred to as entropy stability. The main idea is that we evaluate the projected high-fidelity discretization for an approximation of the current state, assuring entropy stability. Accuracy is retained by locally enriching the tangent space of the nonlinear model reduction space with additional information. Using several numerical experiments we demonstrate that our novel nonlinear and entropy-stable ROMs are suitable for model reduction of systems with strong moving discontinuities and also outperform classical linear model reduction methods.

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MS81

Anatomically Realistic Stochastic Numerical Breast Phantoms for Photoacoustic Virtual Imaging Studies and AI-assisted Image Reconstruction

Photoacoustic computed tomography (PACT) is a non-invasive, radiation-free, low-cost imaging modality that could help identify new biomarkers for early detection of breast cancer, as well as monitoring response to treatment. By combining endogenous hemoglobin optical contrast with ultrasound detection principles, PACT can assess tumor angiogenesis (the formation of new blood vessel structures) and hypoxia (a state of low oxygenation), which result from the increased metabolic activity of aggressively growing malignant breast tumors. However, widespread application of these imaging modalities in a clinical setting requires further investigation. Computer-simulation studies, also known as virtual imaging trials, provide researchers with an economical and convenient route to systematically explore imaging system designs and image reconstruction methods. However, it is essential to employ realistic numerical phantoms that can facilitate the objective, or task-based, assessment of image quality. In this talk, a methodology for producing realistic three-dimensional (3D) numerical breast phantoms for enabling clinically relevant computer-simulation studies of PACT breast imaging is presented. A few case studies will be presented to demonstrate the use of the proposed phantoms to address the development and evaluation of AI-assisted PACT image reconstruction methods.

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MS81

Schwarz-Based Domain Decomposition Solutions for Data-Driven and Physics-Informed Models

Simulating complex physical systems generally requires a modular approach, using separate models to approximate the behavior of subsystems which may be described by different geometries, parameterizations, or governing physics. Joining these separate subsystems often relies on empirical coupling models which may not generalize across all operational regimes. The Schwarz alternating method has been proposed as an alternative to such phenomenological approaches, describing an effective domain decomposition framework which allows for the coupling of arbitrary geometries. In this talk, we present work on combining the Schwarz alternating method with modern data-driven modeling approaches, namely projection-based reduced-order models (PROMs) and physics-informed neural networks (PINNs). This approach can generate surrogates which are capable of simulating advection-dominated fluid flows with higher accuracy and lower cost than comparable monolithic models, aiding analysis in many-query applications such as uncertainty quantification and engi-

neering design. Our methodology for coupling PINNs is demonstrated for the 1D advection-diffusion equation at high Peclet numbers, and results for coupling PROMs are shown for highly non-linear 2D and 3D fluid flows. We explore several nuances of the Schwarz algorithm and their impacts on model performance, specifically the non-overlapping Schwarz approach, additive Schwarz parallelism, and PROM hyper-reduction under domain decomposition.

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MS82

Fokker-Planck-Based Inverse Reinforcement Learning

nverse Reinforcement Learning (IRL) is a compelling technique for revealing the rationale underlying the behavior of autonomous agents. IRL seeks to estimate the unknown reward function of a Markov decision process (MDP) from observed agent trajectories. While most IRL approaches require the transition function to be prescribed or learned a-priori, we present a new IRL method targeting the class of MDPs that follow the Ito dynamics without this requirement. Instead, the transition is inferred in a physics-constrained manner simultaneously with the reward functions from observed trajectories leveraging the mean-field theory described by the Fokker-Planck (FP) equation. We conjecture an isomorphism between the time-discrete FP and MDP that extends beyond the minimization of free energy (in FP) and maximization of the reward (in MDP). This isomorphism allows us to infer the potential function in FP using variational system identification, which consequently allows the evaluation of reward, transition, and policy by leveraging the conjecture. We demonstrate the effectiveness of FP-IRL by applying it to synthetic benchmarks and a biological problem of cancer cell dynamics, where the transition function is unknown.

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MS82

Bayesian Learning and Computation in Single Molecule Data Analysis

The assessment of biological processes at the scales of individual molecules is key to studying life at the level of its most basic elements. Nanoscopy methods, such as STORM, PALM, and PAINT, provide image data directly probing the nanoscale of single molecules. However, it is only after specialized image acquisition protocols are combined with image processing that individual biomolecules are super-resolved at the relevant spatiotemporal scales which, due to light diffraction and Brownian motion, fall far below conventional resolution. As the existing combinations of image acquisition/processing leverage photophysical transitions to distinguish fluorescent molecules from the background, they are largely limited to imaging static specimens. In this talk, I will present a novel image processing framework that does not require photodynamics or additional noise deconvolution, this way allowing for super-resolution imaging of moving specimens. To achieve so, I employ Bayesian nonparametrics and Statistical Learning to develop highly detailed image models that allow for the estimation of single molecule trajectories directly from experimentally obtained raw data. My methods provide estimates with uncertainty propagated from multiple origins including shot and detector noise, pixelation, out-of-focus motion, but most importantly uncertainty propagated from overlapping diffraction limited spots.

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MS82

Online and Parallel Variational Bayesian Inference for Regression and Classification

In this work, the recently introduced sparse online variational Bayesian regression and related models are combined with powerful linear models such as random feature models, and kernel machines to yield inexpensive and scalable alternatives to methods like deep learning. For linear models, the method requires only the iterative parallel solution of deterministic least squares subproblems, on batches of the original data. It is generalized via Laplace approximation to generalized linear models such as multiclass logistic regression. The method is implemented on a range of data sets, where it is shown to compare favourably to some state-of-the-art methods.

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MS82

An Ensemble Score Filter for Tracking High Dimensional Nonlinear Dynamical Systems

We propose an ensemble score filter (EnSF) for solving high-dimensional nonlinear filtering problems with superior accuracy. A major drawback of existing filtering methods, e.g., particle filters or ensemble Kalman filters, is the low accuracy in handling high-dimensional and highly nonlinear problems. EnSF attacks this challenge by exploit-

ing the score-based diffusion model, defined in a pseudo-temporal domain, to characterizing the evolution of the filtering density. EnSF stores the information of the recursively updated filtering density function in the score function, in stead of storing the information in a set of finite Monte Carlo samples. Unlike existing diffusion models that train neural networks to approximate the score function, we develop a training-free score estimation that uses mini-batch-based Monte Carlo estimator to directly approximate the score function at any pseudo-spatial-temporal location, which provides sufficient accuracy in solving high-dimensional nonlinear problems as well as saves tremendous amount of time spent on training neural networks. High-dimensional Lorenz systems are used to demonstrate the performance of our method. EnSF provides surprising performance in reliably and efficiently tracking extremely high-dimensional Lorenz systems (up to 1,000,000 dimension) with highly nonlinear observation processes.

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MS83

Asymptotic Consistency for Nonconvex Risk-Averse Stochastic Optimization with Infinite Dimensional Decision Spaces

Optimal values and solutions of empirical approximations of stochastic optimization problems can be viewed as statistical estimators of their true values. From this perspective, it is important to understand the asymptotic behavior of these estimators as the sample size goes to infinity. This area of study has a long tradition in stochastic programming. However, the literature is lacking consistency analysis for problems in which the decision variables are taken from an infinite dimensional space, which arise in optimal control, scientific machine learning, and statistical estimation. By exploiting the typical problem structures found in these applications that give rise to hidden norm compactness properties for solution sets, we prove consistency results for nonconvex risk-averse stochastic optimization problems formulated in infinite dimensional space. The proof is based on several crucial results from the theory of variational convergence. The theoretical results are demonstrated for several important problem classes arising in the literature.

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MS83

A Low-rank Tensor Method for Risk Averse Optimization

In this talk, we present a low-rank tensor method to solve high-dimensional risk-averse optimization problems governed by partial differential equations (PDEs) under uncertainty. As an example, we focus on the so-called Conditional Value-at-Risk (CVaR), but the approach is equally applicable to other coherent risk measures. We propose an algorithm based on low-rank tensor approximations of random fields discretized using stochastic collocation. To avoid the non-smoothness of the objective function underpinning the CVaR, we consider an adaptive strategy to select the width parameter of the smoothed CVaR to balance the smoothing and tensor approximation errors. Moreover, an unbiased Monte Carlo CVaR estimate can be computed by using the smoothed CVaR as a control variate. The numerical experiments demonstrate that the proposed method enables accurate CVaR optimization constrained by large-scale discretized systems.

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MS83

Towards Optimal Sensor Placement for Inverse Problems in Spaces of Measures

In this talk, we study the identification of a linear combination of point sources from a finite number of measurements. Since the data are typically contaminated by Gaussian noise, a statistical framework for its recovery is considered. It relies on two main ingredients, first, a convex but non-smooth Tikhonov point estimator over the space of Radon measures and, second, a suitable mean-squared error based on its Hellinger-Kantorovich distance to the ground truth. Assuming standard non-degenerate source conditions as well as applying careful linearization arguments, a computable upper bound on the latter is derived. On the one hand, this allows to derive asymptotic convergence results for the mean-squared error of the estimator in the small small variance case. On the other, it paves the way for applying optimal sensor placement approaches to sparse inverse problems.

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MS84

Physics-Informed Stochastic Optimization and Un-

certainty Quantification via Computational-Cost Reduction Methods

We present a multi-objective optimization procedure, for (a) physics-informed design-space dimensionality reduction, (b) adaptive metamodeling, and (c) uncertainty quantification (UQ) based on high-fidelity simulations of seakeeping (operational efficiency and effectiveness) of a destroyer-type vessel. Two hierarchical multi-objectiveproblems are presented, with a level of complexity decreasing from the most general (stochastic sea state, heading, and speed) to the least general (deterministic regular wave, at fixed sea state, heading, and speed). UQ methods include Gaussian quadrature and metamodel-based importance sampling. Numerical simulations are based on unsteady Reynolds-averaged NavierStokes and potential flow solvers.

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MS84

Uncertainty Quantification of Multi-Fidelity Modeling for a Wheel Locomotion System

Prediction of wheeled locomotion performance of planetary rovers poses a significant challenge, mostly due to the complexities of wheel-soil interactions. Consequently, we rely on numerical simulations to predict resulting wheel and system behavior. Different modeling approaches with different levels of fidelity are available. Utilizing multi-fidelity machine learning, we can use abundant low fidelity data and enhance them with a smaller amount of high-fidelity data. This approach can improve prediction accuracy, but also makes it harder to quantify uncertainty of the resulting multi-fidelity model. In the presentation, we will discuss the numerical computation of the propagation of uncertainties through fidelity levels. This includes quantifying the influence of the different numerical solvers on each level. Decoupling uncertainty into computational and mathematical components also offers a promising option. We also discuss how the results can be communicated effectively to operational engineers. As an application, we analyze the case of a locomotion system of an extraterrestrial rover, where uncertainty quantification, uncertainty reduction and a models over- or under-confidence play a critical role.

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MS84

Quantifying Uncertainty in the Outcome of Cardiac Ablation

Radiofrequency catheter ablation (RFA) is a common, minimally invasive procedure to treat cardiac arrhythmias. A catheter is advanced through the patients groin onto a cardiac chamber where the arrhythmogenic tissue is destroyed via electrocautery. Although RFA modeling is a reasonably mature field and Pennes Bioheat equation [Petras A et al, A computational model of open-irrigated radiofrequency catheter ablation accounting for mechanical properties of the cardiac tissue, Int J Num Meth Biomed Engrng 35, 2019] is the standard to describe the power delivery to the tissue, the level of uncertainty in predicting the outcome of a given protocol remains significant. First, the cardiac tissue is highly heterogenous due to the presence of cardiomyocytes, adipose cells and fibroblasts. The other major source of uncertainty is the electrode footprint, namely the contact surface between the catheter tip and the cardiac wall. The electrode footprint is a major determinant to the power actually dissipated in the tissue and depends (among others) on the tip shape, the catheter orientation, and the applied contact force. In addition, during the procedure the patient is sedated, but their heart is beating, which affects the electrode footprint in time, and is yet another source of uncertainty for the whole system. In this talk we will discuss some approaches to account for the inherent variability that exists within the complex biological and procedural aspects of cardiac ablation.

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MS84

Deep Learning Methods for Partial Integrodifferential Equations with Financial Applications

We investigate the use of deep learning approaches for partial integrodifferential equations using stochastic representations of the solutions, combined with simulation procedures. After establishing fundamental properties of the solutions, we develop deep learning algorithms for their approximation, whose performance is compared against that of more traditional numerical methods, such as for instance finite difference methods. The pros and cons of both methods are reported. Applications from the field of financial risk management are considered.

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MS85

Solving Stochastic Inverse Problems with Statistical Scoring

This talk explores a novel approach for solving stochastic inverse problems by quantitatively comparing the distributions of observational and model-generated datasets. This strategy formulates likelihood functions based on statistical scoring, commonly used in forecast verification, to rank parameters in probabilistic models efficiently. We also explore using normalizing flows as density estimators to replace expensive numerical models and neural networks-based nonparametric representations of input functions. These strategies are applied to nuclear physics problems that have been traditionally solved by using histogram or event-binning approaches. The proposed method allows for an unbinned, more accurate, scalable strategy and eliminates biases from histogram partitioning.

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MS85

Bayesian Nonparametric Emulation and Calibration of Climate Models

A climate model (CM) is a set of partial differential equations representing the behavior of the Earth system. For a given input-parameter value, the CM encodes a distribution that is analytically intractable but samples of which can be produced at high computational cost by running the CM with slightly perturbed initial conditions. The goal is to calibrate the CM by finding the parameter value that most closely matches the CM to the true climate distribution. We propose CM calibration via Bayesian optimization using a flexible probabilistic surrogate, which decomposes the joint climate distribution into a sequence of conditional Gaussian-process regressions whose inputs include the CM input parameters. Our framework is scalable and hence it can be applied to large spatial climate fields. We demonstrate the performance of the approach on numerical examples.

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MS85

Calibrated Uncertainty Quantification in Simulator-Based Inference

An open challenge in simulator-based inference (SBI) is how to provide confidence regions of parameters of interest that have a guaranteed probability of including the unknown parameter, regardless of its value and the choice of prior. Related challenges are how to check empirical coverage across the entire parameter space, and how to obtain tighter parameter constraints. Many SBI methods based on posteriors can produce biased or overly confident parameter regions, yielding misleading uncertainty quantification. In this talk, I will present Waldo, a new method that constructs confidence regions with finite-sample validity by leveraging prediction algorithms or posterior estimators that are already widely adopted in SBI. WALDO reframes the well-known Wald test statistic, and uses a computationally efficient regression-based machinery (aka Likelihood-Free Frequentist Inference or LF2I) for classical Neyman inversion of hypothesis tests. I will illustrate the method on examples from high-energy physics and astronomy, and discuss where we stand and what challenges still remain.

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MS86

Conformal Language Modeling

In this work, we propose a novel approach to conformal prediction for generative language models (LMs). Standard conformal prediction produces prediction setsin place of single predictionsthat have rigorous, statistical performance guarantees. LM responses are typically sampled from the models predicted distri- bution over the large, combinatorial output space of natural language. Translating this process to conformal prediction, we calibrate a stopping rule for sampling different outputs from the LM that get added to a growing set of candidates until we are confident that the output set is sufficient. Since some samples may be low-quality, we also simultaneously calibrate and apply a rejection rule for removing candidates from the output set to reduce noise. Similar to conformal prediction, we prove that the sampled set returned by our procedure contains at least one acceptable answer with high probability, while still being empirically precise (i.e., small) on average. Furthermore, within this set of candidate responses, we show that we can also accurately identify subsets of individual componentssuch as phrases or sentencesthat are each independently correct (e.g., that are not hallucinations), again with statistical guarantees. We demonstrate the promise of our approach on multiple tasks in open-domain question answering, text summarization, and radiology report generation using different LM variants.

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MS86

Foundation Models for Robust Design of Biological Systems

Engineering biological systems to precise specifications can be a daunting task one that requires the ability to tackle vast design spaces emerging from the diversity in the biophysical and biochemical mechanisms and one that also requires certain ingenuity in understanding the genetic basis of how such mechanisms emerge. In this talk, I will outline a paradigm where we posit that autonomous discovery i.e., automated labs that are managed and run using artificial intelligence (AI) techniques can vastly benefit biological design applications. Further, to tackle the complexity of biological design, we argue that a specific class of AI techniques, namely foundation models – unsupervised

learning techniques that can summarize vast troves of rich biological data can outperform classical techniques. We illustrate this paradigm of using foundation models and autonomous discovery on three exemplar applications: (1) designing antimicrobial peptides using generative models; (2) engineering proteins using genome-scale language models; and (3) understanding the basis of how SARS-CoV-2 may evolve into new variants of concern. Our work demonstrates that AI-based generative models and autonomous discovery holds much promise for how we can engineer novel biological systems. We also articulate challenges that emerge from integrating diverse robotic platforms within the context of autonomous discovery and discuss how these challenges can be overcome

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MS86

Simple Baselines for Uncertainty Quantification and Conformal Calibration for Black Box LLMs

Large language models (LLMs) specializing in natural language generation (NLG) have recently started exhibiting promising capabilities across a variety of domains. However, gauging the trustworthiness of responses generated by LLMs remains an open challenge, with limited research on uncertainty quantification for NLG. Furthermore, existing literature typically assumes white-box access to language models, which is becoming unrealistic either due to the closed-source nature of the latest LLMs or due to computational constraints. In this work, we investigate uncertainty quantification in NLG for black-box LLMs. We first differentiate two closely-related notions: uncertainty, which depends only on the input, and confidence, which additionally depends on the generated response. We then propose and compare several confidence/uncertainty metrics, applying them to selective NLG, where unreliable results could either be ignored or yielded for further assessment. Our findings on several popular LLMs and datasets reveal that a simple yet effective metric for the average semantic dispersion can be a reliable predictor of the quality of LLM responses. This study can provide valuable insights for practitioners on uncertainty management when adopting LLMs.

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MS87

Solving Inverse Problems with Noisy Measurements via Deep Orthogonal Decomposition

Inverse problems are notoriously difficult to address, mainly because of their ill-posedness and because of the elevated computational cost required for their solution. A classic example concerns reconstructing the state of a given system, such as the solution to a parameter dependent differential problem, through a collection of (noisy) measurements, as in tomographic reconstruction [Arridge et al. (2006), Approximation errors and model reduction with an application in optical diffusion tomography] or damage detection [Rosafalco et al. (2021), Online structural health monitoring by model order reduction and deep learning algorithms]. Here, we propose a technique based on a novel deep learning approach termed Deep Orthogonal Decomposition (DOD), where a deep neural network is used to describe the solution manifold, that is the collection of all possible configurations of the systems state, through a continuously adaptive local basis. The idea is that the DOD associates a local subspace of possible sensor measurements to each state of the system: then, this knowledge can be used to solve the corresponding inverse problem without intrusive/expensive calls to the forward operator. Additionally, the approach is extremely flexible as it allows us to handle a variable number of (noisy) observations, going from pointwise evaluations (sensor data) to macroscale functionals (e.g., spatial average of the solution field).

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MS87

Reduced Order Models and Bayesian Approaches for the Solution of Inverse Heat Conduction Problems

Accurate real-time estimation of the heat flux at the interface between the Continuous Casting (CC) mold and molten steel is imperative for the smooth operation of CC machinery. In this context, a stochastic inverse heat transfer problem (IHTP) is formulated to infer the transient heat flux, treated as an unknown Neumann boundary condition. Therefore, an Ensemble-based Simultaneous Input and State Filtering (EnSISF) as a Data Assimilation (DA) technique incorporating Radial Basis Functions (RBFs) to enhance computational efficiency is utilized for simultaneous temperature distribution prediction and heat flux estimation. The procedure is based on the sequential availability of temperature provided by thermocouples inside the mold. Our research contributes significantly to achieving probabilistic boundary condition estimation in real-time, handling noisy measurements and errors in the model. This paves the way for efficient real-time monitoring and control, which is critical for preventing caster shutdowns.

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MS87

SINDy-RL: Uncertainty-Aware Active Learning for Simultaneous Dynamics Discovery and Control

Modern dynamics discovery and control design techniques

have been essential for the rapid advancement of science and technology across a multitude of domains. In particular, deep reinforcement learning (RL) has shown significant promise for uncovering sophisticated control strategies in complex environments. However, these strategies often require millions of interactions in the environment to train neural network policies, which may be infeasible for systems where data collection is expensive. While access to a sufficiently accurate surrogate model can greatly reduce the number of interactions with an environment, obtaining such a model can become difficult in data-limited settings where there may be significant uncertainty in the dynamics. In this work, we propose a novel approach using the Sparse Identification of Nonlinear Dynamics (SINDy) to simultaneously (1) construct interpretable models of the environment dynamics, (2) quantify the uncertainty of the dynamics model, and (3) utilize the uncertainty to design controllers for the system. By applying our techniques to mechanical and fluid systems with limited data, we investigate the trade-off between exploiting the learned dynamics model to improve the control objective and using the uncertainty to inform additional data collection from the environment to improve our model.

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MS88

Robust Optimal Experimental Design for Nonlinear Inverse Problems

An optimal experimental design (OED) can be defined as the design/control that maximizes a predefined utility function (or alternatively the one that minimizes some optimality criterion). OED is quickly evolving to be an indispensable tool for optimizing data acquisition for large-scale and expensive scientific simulations and experiments in a wide range of applications such as sensor placement and trajectory planning. OED for nonlinear inverse problems is faced by challenges including the choice of the utility function, inherent binary/discrete nature of the design which yields nonsmoothness of the optimization objective, and the prohibitive computational cost of traditional numerical optimization algorithms typically employed to solve a relaxed/approximate version of the original OED optimization problem. Moreover, OED mathematical formulations and solution approaches generally overlook misspecification of the elements of the inverse problem such as the prior and the measurement uncertainties. In this talk, we present mathematically robust and efficient recipes for solving binary OED optimization problems resulting from nonlinear inverse problems with potentially black-box utility functions, such that the optimal design is robust with respect to misspecification of elements of the inverse problem.

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MS88

Non-Isomorphic D- and A-Optimal Main-Effects Designs

For run sizes that are a multiple of four, the literature offers many two-level designs that are D- and A-optimal for the main-effects model and, given this feature, minimize the aliasing between main effects and interaction effects and among interaction effects. For run sizes that are not a multiple of four, no conclusive results are known. In this paper, we propose algorithms that generate all non-isomorphic D- and A-optimal main-effects designs for run sizes that are one and two more than a multiple of four. We enumerate all such designs for run sizes up to 18, report the numbers of designs we obtained and compare the minimally aliased designs we found with benchmark designs from the literature.

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MS88

Stability of Bayesian Optimal Experimental Design

We discuss stability of the expected utility in Bayesian optimal experimental design under different model perturbations. In particular, we focus to the context of high-dimensional inverse problems. The stability analysis gives rise to new approximation schemes for which we demonstrate fast convergence rates.

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MS88

Perspective on Multiple Facets of Modern Experimental Design

Optimum experimental design (OED) is the area of statistical methodology concerned with the optimal capture of information to build reliable models in numerous areas of science, technology and commerce. The prospective measurement data are then to be used to infer unknown model parameters. OED means careful setting of controllable input variables, or factors, decisions about the best

sensor location, choices of which units to treat, etc. Without this effort there might be huge losses in haphazard decisions about data capture, as one may just be looking in the wrong place for the answer or not be able to measure key causal effects. OED has applications in many fields where experiments are done to develop new theories or to confirm existing hypotheses. However, it may be challenging due to high-dimensionality of parameters, correlations among measurements, model error, additional modeling uncertainties, or high cost of evaluating the model. What is more, researchers in different fields tend to become specialized, to use different vocabulary for the same thing, and to reinvent the same ideas, unaware that they have already been developed in another area. In this work, we will examine several representative applications of OED and review different areas of methodology which will be discussed in this minisymposium. The fragmentation in the subject and strong links with other parts of mathematics, such as algebra, combinatorics, optimization will also be discussed.

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MS89

Dynamic Mode Decomposition for Source Identification

Identification of sources of groundwater contamination is a crucial component of the design of effective remediation actions. This inverse-modeling task, which involves estimation of both locations of contaminant release and its temporal history, must contend with sparse (in space and time) observations of subsurface solute concentration. Subsurface heterogeneity and data scarcity translate into computationally expensive probabilistic inverse problems solved, e.g., via Markov chain Monte Carlo. We propose the use of dynamic mode decomposition (DMD) as an alternative tool for contaminant source identification. DMD discerns dominant patterns in the dynamical systems behavior, directly from snapshots of the system evolution, and then generates a reduced-order model for the computationally efficient prediction of the temporal evolution of the system states. Grounded in singular value decomposition, DMD is a regression of spatially distributed data, collected from a dynamical system at multiple times, onto locally linear dynamics. We investigate the efficiency of the method on a synthetic contaminant source identification problem.

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MS89

A Stochastic Investigation of Bifurcating Phenomena in Computational Fluid Dynamics

Incorporating probabilistic terms in mathematical models is crucial for capturing and quantifying uncertainties in real-world systems. Indeed, randomness can have a significant impact on the solution behavior, and more realistic and informative results can thus be obtained. On the other hand, the simulation of stochastic models can require significant computational resources due to the need to generate numerous realizations of the system. This makes the development of reduction tools, such as surrogate models, essential for enabling efficient and scalable simulations. In this work, we show a preliminary investigation of bifurcating phenomena originating in fluid dynamics, namely the Coanda effect. We exploit polynomial chaos expansion (PCE) studying the accuracy of surrogate representations to given stochastic processes. Then, its inclusion in the finite element (FE) setting is described, arriving at the formulation of the enhanced stochastic FE method. Moreover, we introduce Bayesian inference in the framework, providing a posterior knowledge of the probabilistic solution, capable of producing a powerful setting for hyper-parameters learning and model fidelity comparison.

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MS89

Adaptive Collocation-Based Approximation of Parametric Nonlinear Eigenproblems

When dealing with complex dynamical systems, the solution of eigenvalue problems is pivotal in the analysis of frequency responses and in controller design. Eigenvalue nonlinearities can easily arise, e.g., when dealing with controller delays. Moreover, parameters are often included to model uncertainties or design variables. In this context, we propose a strategy for solving parametric nonlinear eigenproblems. For a wider applicability of our method, we stay non-intrusive: we make no assumptions on how the problem depends on the eigenvalue or on the parameters. Our method piggybacks on a reliable contour-integration-based eigensolver for dealing with *non-parametric* versions of the target problem, obtained by "freezing' all parameters at some collocation parameter values. Then the collection of obtained eigenvalues is used to synthesize the *eigenvalue manifolds*, i.e., to understand how the eigenvalues vary as the parameters change. Several issues arise, mostly due to the possible irregularity in the eigenvalue manifolds: (i) manifold crossings may happen if the target spectrum is not well isolated, (ii) bifurcations may reduce the smoothness of the manifolds, and (iii) the target manifolds may "appear and disappear' as parameters vary, since eigenvalues may migrate outside the integration contour. We describe a strategy to flag these undesirable effects, and, to some extent, to circumvent them.

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MS90

Optimization-based Frequentist Confidence Intervals for Functionals in Constrained Inverse Problems: Resolving the Burrus Conjecture

We introduce an optimization-based framework to construct confidence intervals for functionals in constrained inverse problems, ensuring valid one-at-a-time frequentist coverage guarantees. Our method builds upon the now-called strict bounds intervals which offer ways to directly incorporate any side information about parameters during inference without introducing external biases. By tying these intervals to an inversion of a constrained likelihood ratio test, we translate interval coverage guarantees into type-I error control, and characterize the resulting interval via solutions of optimization problems. Along the way, we refute the Burrus conjecture. Our framework provides a novel approach to analyze the conjecture and construct a counterexample by employing a stochastic dominance argument, which we also use to disprove a general form of the conjecture. We illustrate our framework with several numerical examples and provide directions for extensions beyond the Rust–Burrus method for non-linear, non-Gaussian settings with general constraints.

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MS90

Extending Normalizing Flows to Propagate Uncertainty in Neural ODEs

Predictions for continuous-time dynamical systems may be subject to several interacting sources of uncertainty. In a system where dynamical noise is assumed to be present, a predictive model must account for both the randomness of the initial state of an input and the sensitivity of the employed differential equation solver. We propose a prediction pipeline which efficiently quantifies predictive uncertainty for real dynamical data. The pipeline firstly entails training a neural ODE to learn the underlying dynamics of the generating system. Secondly, a flow-based model which extends the normalizing flow model is developed to learn a time series of densities which propagates the assumed initial state noise information under the learned dynamics. We then demonstrate this pipeline for performing predictive uncertainty quantification using some real time series data

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MS90

Uncertainty Quantification for a Bacterial Hybrid Promoter Library

Bacterial gene expression is often modelled using ordinary differential equations. These models contain unknown parameters which are estimated by fitting models to experimental data. Naturally, the resulting parameter estimates have uncertainty which can be quantified in several ways, each with their own tradeoffs. It is important to quantify both parameter and prediction uncertainties during the process of model validation. Previously, we heavily motivated using time-dependent model characteristics and time-varying nonlinear models for genetic circuits. We continue this motif in the context of uncertainty quantification via time-series biological data from a novel library of promoters. Different types of promoters exist such as one that encodes for gene activation while the cell population is in growth phase, and one for gene activation during stationary phase. We have stitched together a growth phase promoter and a stationary phase promoter to create a hybrid promoter, implying that it should exhibit different types of gene expression during the cell populations life cycle. We then created several mutated variants of this promoter to create a library of hybrid promoters in which each hybrid promoter has distinct gene expression profiles during the 2 targeted phases of the life cycle. Once we have our hybrid promoter library, we analyze the parameter and prediction uncertainties associated with these promoters in different genetic circuit contexts.

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MS90

Surrogate Based Black-box Optimization with Polynomial Model Based-Optimization (PMBO)

Optimization tasks arise in many fields of applications, ranging from analyzing and adjusting simulations of complex systems to inferring optimal neural network architectures. The (hyper-) parameters of such systems are to be adjusted such that a predefined objective function is minimized. PMBO is a novel black-box optimizer that does not only find the minimum of the objective function but also provides - by fitting a polynomial surrogate to the objective function - additional information about the search space. An acquisition is introduced which proposes the next sample point, balancing exploration and exploitation of the search. Since the surrogate is a polynomial, analysis of the model, including integration and differentiation, is far easier than for a fitted distribution. PMBO is benchmarked against other state-of-the-art algorithms given a set of artificial, analytical functions provided by the Black-box Optimization Benchmarking (BBOB) test suit.

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MS91

StructuredMaps: a package for gradient-based dimension reduction and measure transport for Bayesian inverse problems

Inference is a pervasive task in science and engineering applications. The Bayesian approach to inference facilitates informed decision-making by quantifying uncertainty in parameters and predictions but can be computationally demanding. In the case of Bayesian methods for inverse problems governed by partial differential equations (PDEs), the high dimensionality of model parameters and data can render nave posterior exploration intractable. In this talk, we present StructuredMaps, a Python package for

1) discovering low-dimensional structure in PDE-governed inverse problems, and 2) exploiting such structure to perform inference efficiently using measure transport. StructuredMaps implements several gradient-based dimension reduction methods motivated by a priori error bounds between the posterior distribution and its approximation. The discovered low-dimensional structure is then encoded into the parameterization of a transport map, a mapping between the target posterior distribution and a simple reference distribution (e.g., a standard Gaussian). We present dimension reduction and inference results for inverse problems related to steady-state Darcy flow and inverse scattering.

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MS91

Multi-Output Multilevel Best Linear Unbiased Estimators Via Semi-Definite Programming

Multifidelity forward uncertainty quantification (UQ) problems often involve multiple quantities of interest and heterogeneous models (e.g. different grids, equations, dimensions, physics, surrogate and reduced-order models). While computational efficiency is key in this context, multi-output strategies in multilevel/multifidelity methods are either sub-optimal or non-existent. In this paper we extend multilevel best linear unbiased estimators (MLBLUE) to multi-output forward UQ problems and we present new semidefinite programming formulations for their optimal setup. Not only do these formulations yield the optimal number of samples required, but also the optimal selection of low-fidelity models to use. While the existing MLBLUE approaches are single-output only and require a non-trivial nonlinear optimization procedure, the new multi-output formulations can be solved reliably and efficiently. We demonstrate the efficacy of the new methods and formulations in practical UQ problems with model heterogeneity.

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MS91

Extensions and Open-Source Algorithms for Data-Driven Modeling with Dynamic Mode Decomposition

The dynamic mode decomposition (DMD) is a powerful data-driven modeling technique that reveals coherent spatiotemporal structures and produces future-state predictions from data. The methods simple linear algebra-based formulation additionally allows for various optimizations and extensions that make the algorithm more practical and viable for analyzing real-world data. As a result, DMD has grown to become a leading method for equation-free system modeling across multiple scientific disciplines. PyDMD is a Python package that implements DMD and several of its most prominent variants. In this talk, I discuss the current functionalities of the PyDMD package, while also providing an overview of our recent work to incorporate various cutting-edge DMD methods and tools into PyDMD. I will discuss the theory behind several modern DMD innovations and provide users with practical tips. I will additionally demonstrate how one might use PyDMD in order to model and analyze real-world data sets.

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MS91

PyApprox: a Software Package for Sensitivity Analysis, Bayesian Inference, Optimal Experimental Design, and Multi-fidelity Uncertainty Quantification and Surrogate Modeling

PyApprox is a Python software package that provides flexible and efficient tools for credible data-informed decision making. PyApprox implements methods addressing various issues surrounding high-dimensional parameter spaces and limited evaluations of expensive simulation models with the goal of facilitating simulation-aided knowledge discovery, prediction and design. This talk will provide an overview of the various methods available in PyApprox for surrogate modeling, sensitivity analysis, uncertainty quantification, optimal experimental design and risk

assessment. Focus will be given to automated tools that do not require extensive hand-tuning of hyper-parameters. The methods overview will be complemented by various numerical examples that demonstrate the plug an play nature of PyApprox which is designed to allow rapid prototyping and comparison of existing methods.

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MS92

Coupling a Climate and Ice Sheet Model with Emulation

Asynchronous coupled climate and ice-sheet computer models are used to study atmosphere and ice-sheet interactions and guide policy decisions. However, their direct use is inhibited by: their complex structure; high-dimensional input and output spaces including spatial-temporal fields; and their long evaluation times. Surface Mass Balance (SMB); the difference in ice accumulation from snowfall and loss due to melting and other processes, is an output of the substantially more computationally expensive climate model which is input to the quick to evaluate ice-sheet model. This severely limits the number of simulations necessitating an emulator for SMB. However, SMB is an incomplete spatial field which is only returned by the climate model in grid cells where there is a positive surface ice fraction. Each simulation and time-step thus yields a different shaped SMB spatial field dependent on the current ice-sheet profile. These challenges render standard multivariate and spatial field emulation techniques inadequate. We develop SMB-Gen, a novel Bayesian emulator exploiting a latent Gaussian process model to mitigate these challenges and couple this to an ice-sheet model. This is applied to the FAMOUS-Glimmer model for the North American ice-sheet during the last glacial maximum. This enables a large number of model evaluations to perform an uncertainty quantification to constrain projections of ice-sheet instabilities and obtain robust estimates of future sea level rise.

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MS92

Decision Support with Digital Twins as an Inverse Problem with Application to Net Zero Policy Making

One critical component of the recent interest in "Digital Twins" and digital twinning technology is their use to assist in decision making. Suppose we consider a digital twin to combine process-based simulation modelling with frequently updating data streams, so that the twin can learn and respond to changes in the data. How might one then use that system in decision support? For this talk we consider the twin as a complex function of parameterised decisions and argue that decision support can be conceptualised as an inverse problem. We compare that to the traditional use of models for decision support, either providing simulations at a handful of user-chosen scenarios, or optimising within parameter space to find a "best decision". We argue that both approaches are likely ineffective for real decision makers. We present our methods using digital twins being developed for policy makers considering how to incentivise tree planting in the UK's drive towards Net Zero whilst enhancing biodiversity, water quality and other ecosystem services. We show that our methods deliver an explorable space of policy options that are compatible with targets on Greenhouse Gas removal, food security and biodiversity loss and yet that deliver quite different spatial distribution of planting. We demonstrate how real-time preference elicitation can enable a user to explore different target compatible options within these digital twins.

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MS92

Probability-Free Digital Twinning Using Linked Bayes Linear Emulators with Uncertain Inputs.

Computationally expensive simulators, implementing mathematical models in computer codes, are commonly approximated using statistical emulators. We develop and assess novel methods for approximating systems best modelled via a chain, series or network of simulators. In particular, we consider this task within a Bayes linear framework, where the approximated output (expectation) and uncertainty estimate (variance) for one emulator becomes the input a subsequent emulator, thus being able to explicitly account for simulator input uncertainty induced by links between models in arbitrarily large networks. We demonstrate the advantages of this method compared to i) use of a single emulator of the composite simulator network; and ii) a sampling approach derived from the individual Bayes linear second order approximations for each simulator. These comparisons are presented in the context of the motivating application of an epidemiological simulator chain to model the impact of an airborne infectious disease.

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MS94

History Matching in High Dimensions

History Matching is a class of algorithms treating inverse problems, often used in industry for calibrating complex models in place of, or in conjunction with, more expensive MCMC methods. For large models, parsimonious algorithms commonly exploit Gaussian process emulation as a method of surrogate modelling. Our work explores more cost-effective methods for constructing emulators in high dimensions, further extending the versatility of History Matching.

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MS94

Ensemble Feedback Stabilization of Linear Systems

A Riccati-based feedback mechanism is analyzed for stabilization of linear control systems with parameter-dependent system matrices. The feedback is constructed by means of a finite ensemble of parameters from a training set. Conditions are provided under which this feedback law stabilizes all systems of the training set and also systems in its vicinity. Moreover, its suboptimality with respect to the optimal feedback for each single parameter from the training set can be quantified. The theoretical findings are illustrated with a set of application-motivated examples and confirming numerical experiments.

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MS94

Thresholded Estimation of Covariance Operators and Application in Ensemble Kalman Methods

Covariance operator estimation is a fundamental task which arises in many particle methods for data assimilation. This talk introduces a notion of sparsity for infinite-dimensional covariance operators and a family of thresholded estimators which exploits it. In a small lengthscale regime, we show that thresholded estimators achieve an exponential improvement in sample complexity over the standard sample covariance estimator. Our analysis explains the importance of using covariance localization techniques in ensemble Kalman methods for global data assimilation.

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MS94

Novel Localisation for Ensemble Data Assimilation

High dimensional Bayesian inference problems require immense computation time and still pose a significant challenge. Filters based on Monte Carlo type ensemble approximations of the corresponding posterior distribution are considered state of the art. Yet for these filters robustness in combination with computational feasibility is typically achieved via the assumption that the posterior belongs to a parametric family of densities, e.g. is a Gaussian. While consistency in the ensemble can only be realized without such limiting restrictions on the filter, feasibility and robustness can often not be maintained in that case. Here we propose a novel localization scheme to stabilize the ensemble based filters.

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MS95

A Novel Approach for Sampling Isotropic Gaussian Random Fields

Generating realisations of Gaussian random fields is an important step in a variety of methods for the solution of Bayesian Inverse Problems. For instance, Gaussian random fields often correspond to a choice of prior measure, or enter the computation of likelihoods through parameters of a stochastic partial differential equation. Many common sampling techniques reach their limits in settings, where the random field needs to be evaluated at a large number of points and the random field has low regularity or short correlation length. We propose a sampling method which is able to quickly and accurately compute realisations of isotropic Gaussian random fields in these situations. To this end, a suitable periodisation of the covariance function is evaluated by means of a combination of Discrete Cosine and Discrete Sine Transforms. We provide explicit error bounds for the covariance of the resulting process. Furthermore, we use a link between our method and sampling approaches based on stochastic partial differential equations, to investigate the issue of boundary artifacts arising in those methods.

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MS95

Enabling Efficient and Scalable Bayesian Inversion with Derivative-Informed Neural Operators

Scalable and efficient methods for the solution of infinite-dimensional Bayesian inverse problems require derivative information of e.g., a likelihood function. These algorithms are very query intensive, limiting their application in settings where derivative computations are expensive. In this talk, we will present efficient methods for learning derivatives of parametric PDE maps on function spaces via derivative-informed neural operators (DINOs). Once these DINOs are constructed online derivative computations can be made inexpensive, enabling fast solution of Bayesian inverse problems via derivative-based methods. We will demonstrate results using geometric MCMC methods as well as transport methods, which both require derivatives of the PDE map.

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Early Stopping for Bayesian Linear Inverse Problems

This talk is focused on linear Bayesian inverse problems, and its main goal is implementing and analyzing an adaptive data dependent method to choose the scale parameter of a Gaussian prior. The method we study arises from early stopping methods, which have been successfully applied to a range of problems for statistical inverse problems in the frequentist setting. We study the use of a discrepancy based stopping rule, in the setting of random noise. We show that this stopping rule results in optimal rates under certain conditions on the prior covariance operator. We further derive for which class of signals this method is adaptive. It is also shown that the associated posterior contracts at the optimal rate and provides a measure of uncertainty. We demonstrate the theoretical results using the Ensemble Kalman filter (EnKF) by which the choice of the regularization parameter is shown to be equivalent to choosing a stopping time.

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MS96

Systematic Parameter Calibration with Machine Learning-Based Emulation of a Global Land Model

Land models simulate societally relevant processes such as ecosystem dynamics, terrestrial hydrology, and agriculture with a high degree of complexity. Adequately predicting terrestrial processes such as climate-carbon feedbacks relies on assessing confidence in these models and their predictive capabilities while minimizing sources of model error. Full complexity land models include a large number of parameters that determine fluxes and states predicted by the model. Automated and systematic land model parameter calibration is hindered by, among other factors, interacting process complexity, large and poorly constrained parameter spaces, and prohibitive computational costs for spin-up and model ensembles. A machine learning approach to model calibration can provide increased computational efficiency and reduced analysis time as well as objective methods to assess calibration results. Here we use a variety of statistical and machine learning approaches to emulate parameter response functions in the Community Land Model, version 5, and calibrate the global model. By sampling from the plausible parameter space and running future climate simulations, we can estimate the contribution of parametric uncertainty on emergent features of the climate system such as the trajectory of the land carbon sink.

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MS96

A Partitioned Sparse Variational Gaussian Process for Fast, Distributed Spatial Modeling

The next generation of Department of Energy supercomputers will be capable of exascale computation. As a result, users will be unable to rely on post-hoc access to data for uncertainty quantification and other statistical analyses and there will be an urgent need for sophisticated machine learning algorithms which can be trained in situ. Algorithms deployed in this setting must be highly scalable, memory efficient and capable of handling data which is distributed across nodes as spatially contiguous partitions. One suitable approach involves fitting a sparse variational Gaussian process (SVGP) model independently and in parallel to each spatial partition. The resulting model is scalable, efficient and generally accurate, but produces the undesirable effect of constructing discontinuous response surfaces due to the disagreement between neighboring models at their shared boundary. In this paper, we extend this idea by allowing for a small amount of communication between neighboring spatial partitions which encourages better alignment of the local models, leading to smoother spatial predictions and a better fit in general. Due to our decentralized communication scheme, the proposed extension remains highly scalable and adds very little overhead in terms of computation (and none, in terms of memory). We demonstrate this Partitioned SVGP (PSVGP) approach for the Energy Exascale Earth System Model (E3SM) and compare the results to the independent SVGP case.

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MS96

Uncertainty Quantification of Regional Antarctic Ice Sheet Dynamics Using High-resolution Model Ensembles

The Antarctic ice sheet is an uncertain and potentially large contributor to future sea level rise projections. Uncertainties in future ocean and atmospheric warming, ice dynamics and thermodynamics, and initial and topographic boundary conditions combine with marine ice shelf dynamics, calving, hydrology, and other processes to produce a wide spread of potential ice discharge scenarios. We discuss the application of perturbed-parameter ensembles to high-resolution regional Antarctic ice sheet glacier modeling. We outline an uncertainty quantification approach to calibrating simulations and projecting quantities of interest such as sea level rise, involving statistical machine learning methods for computer model emulation and Bayesian parameter estimation.

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MS96

Conditional Generative Models for Efficient Uncertainty Quantification with Application in Climate Models

We propose a score-based generative sampling method for solving the amortized Bayesian inference problem. Estimating uncertainty in nonlinear inverse problems is computationally expensive. For example, a Markov chain Monte Carlo (MCMC) sampling typically requires hundreds of thousands, or even millions of model evaluations to get convergence and these model simulations cannot be done fully in parallel. To overcome this issue, we incorporate the score-based diffusion model into the Bayesian inference framework to develop a novel score-based conditional generative model. The key idea is to store the information of the posterior density function in the score function, in stead of storing the information in a set of finite Monte Carlo samples. By leveraging the reverse-time diffusion process, the proposed generative model can generate unlimited samples to characterize the posterior density. An essential aspect of our method is its analytical update step, gradually incorporating data information into the score function. We demonstrate our method in both synthetic and real-data applications. Results indicate that our method can produce accurate parameter posterior distributions similar to MCMC sampling and it generates model outputs close to the E3SM land model (ELM) simulations. Additionally, both the inverse and forward evaluations are computationally efficient which allows for rapid integration of observations for parameter estimation and fast model predictions.

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MS97

Low-Rank Posterior Approximations for Linear Gaussian Inverse Problems on Separable Hilbert Spaces

In Bayesian inverse problems, the computation of the posterior distribution can be computationally demanding, especially in many-query settings such as filtering, where a new posterior distribution must be computed many times. When doing inference on a function, the parameter is moreover infinite-dimensional. In this work we consider some computationally efficient approximations of the posterior distribution for linear Gaussian inverse problems defined on separable Hilbert spaces. We measure the quality of these approximations using, among others, the Kullback-Leibler divergence of the approximate posterior with respect to the true posterior and investigate their optimality properties. The approximation method exploits low dimensional behaviour of the update from prior to posterior, originating from a combination of prior smoothing, forward smoothing, measurement error and limited number of observations, analogous to the results of [Spantini et al., SIAM J. Sci. Comput. 2015] for finite dimensional parameter spaces. Since the data is only informative on a low dimensional subspace of the parameter space, the approximation class we consider for the posterior covariance consists of suitable low rank updates of the prior. In the Hilbert space setting, care must be taken, such as when inverting covariance operators. We address such challenges by using the Feldman-Hajek theorem for Gaussian measures.

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MS97

Choosing Observations to Mitigate Model Error in Bayesian Inverse Problems

In inverse problems, one often assumes a model for how the data is generated from the underlying parameter of interest. In experimental design, the goal is to choose observations to reduce uncertainty in the parameter. When the true model is unknown or expensive, an approximate

model is used that has nonzero 'model error' with respect to the true data-generating model. Model error can lead to biased parameter estimates. If the bias is large, uncertainty reduction around the estimate is undesirable. This raises the need for experimental design that takes model error into account. We present a framework for model error-aware experimental design in Bayesian inverse problems. Our framework is based on Lipschitz stability results for the posterior with respect to model perturbations. We use our framework to show how one can combine experimental design with models of the model error in order to improve the results of inference.

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MS97

Bayesian Inference of Discretely Observed Diffusions

We consider the inverse problem of recovering the diffusion and drift functions of a stochastic differential equation from discrete measurements of its solution. We show the stability of the posterior measure with respect to appropriate approximations of the underlying forward model allowing for priors with unbounded support. Then, in the case where the diffusion coefficient is small, we look at Gaussian approximations of the transition densities and the resulting approximated posterior. This is based on joint work with J.-C. Croix, S. Katsarakis, I. Kiss and T. Zerenner.

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MS98

Surrogate Modeling for Scalable Fast Time-to-Solution Model Exploration of Stochastic Simulations

The COVID-19 pandemic highlighted the roles that epidemiological models can play in supporting decision making in times of crisis. For epidemiological models to be useful in producing forward projections or running what-if scenarios they need to be calibrated to empirical data. However, many epidemiological models employ stochasticity to capture limits in our ability to know with certainty the fundamental processes driving epidemiological dynamics. This impacts what is meant by calibration, as empirical data gets compared to an ensemble of models, where each member of the ensemble is mapped to a specific model trajectory, defined as a combination of a model input parameter set and a random seed. Most calibration approaches used for stochastic simulations attempt to match the mean behavior of a model, or some other summary statistics, to empirical data. In this talk we will present a calibration framework that seeks to explicitly emulate the individual model trajectories, using common random numbers (CRN). This Trajectory Oriented Optimization (TOO) approach uses CRN-based Gaussian process surrogates within a Thompson sampling scheme to efficiently find optimal model trajectories. We will compare and contrast the TOO approach to other calibration approaches using stochastic epidemiological models. We will also describe computational and numerical techniques that make this approach feasible to be used in time sensitive use cases such as emerging public health emergencies.

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MS98

Predicting Performance Variability of Ignition Experiments at the NIF with Machine Learning

Recent experiments at the National Ignition Facility (NIF) in Livermore, California have demonstrated fusion breakeven where the energy produced from hydrogen fusion exceeds the laser energy used to initiate the reactions for the first time. The experiments were also the first in which a data-driven model was used to predict the outcome before the NIF laser was fired. The success of our Bayesian predictive model, both in correctly predicting the outcome of ignition experiments and in matching the fast pace of experimental work at the NIF, relies on our joint use of experimental and simulation datasets, deep neural network surrogate models, and transfer learning to accelerate the training of new models. In this talk we will present our Bayesian predictive model, its applica0on to igniting fusion experiments, and discuss the use of deep surrogates trained on large ensembles of high-fidelity radiation hydrodynamics simulations as an essen0al enabling technology. We will present the architectures we have developed for production-scale development of deep surrogates and our use of transfer learning, which reduces the computa0onal overhead for training new models by 100-1000 times. Finally, we will present new opportunities for the validation of our large-scale simula0on codes using NIF data that our data-driven approach has enabled. Prepared by LLNL under Contract DE-AC52-07NA27344. LLNL-ABS-858207

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MS98

Working at the Intersection of Projection-Based Reduced-Order Models, UQ, and HPC. A Tale of How to Make Virtue Out of Necessity

Scientific research typically involves identifying a problem of interest, developing a (mathematical) formulation and, if analytical solutions are unfeasible, resorting to numerical ones. Sometimes, these stages are disconnected, for example when the formulation is carried out in a "bubble" without keeping into consideration the numerical solution aspect, or the final use case. This "compartmentalization" can lead to misleading conclusions about the feasibility or value of a formulation, since only limited metrics are considered. In this talk, I will present one example in the context of projection-based reduced-order models (pROMs). A common denominator of most works on pROMs has been and still is the search for the smallest approximation space (e.g., number of modes) suitable for a target problem. This is motivated by the idea that "the smaller the subspace, the better". This fits the limitation mentioned above. I will argue that a large subspace is, for some problems, not only necessary for accuracy, but can also benefit computational efficiency. Specifically, I will focus on linear time-invariant systems, for which pROMs can be considered very mature in terms of methodological and theoretical development. I will discuss various aspects to support my statement, and finally show some results from the simulation of elastic seismic shear waves.

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MS98

Optimally Transported Meshes for Model Reduction and Uncertainty Quantification of High Speed Flow

We present an r-adaptive mesh adaptation method that aids in the high-fidelity simulation of parametric compressible flow problems and in the construction of reduced-order models. Starting from a fixed reference mesh, grid nodes are redistributed via solutions of the Monge-Ampre equation in order to concentrate the mesh towards features that require more resolution. When repeatedly solving for high-fidelity simulations at different values of uncertain parameters, this process allows for mesh adaptation without changing the grid topology for each simulation. The solution flow fields can be mapped back onto the starting reference mesh. On the reference mesh, sharp and local features like parametrically varying shocks are smoothed out and brought into closer alignment. Projection-based reduced-order models are then constructed for the solution field and mesh mapping. These reduced-order models can then be used to speed up methods for forward uncertainty propagation. This approach is applied to two-dimensional supersonic and hypersonic flow problems with uncertain boundary conditions.

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MS99

Extending Multi-Fidelity Modelling to Stochastic Simulators

Multi-fidelity surrogate models (MFSMs) fuse information from models with varying computational fidelities into a new surrogate model (SM). Such models can predict the output of complex systems with a higher accuracy and lower cost compared to single-fidelity SMs. MFSMs can be constructed based on high- and lower-fidelity data from physical experiments and/or computer simulations. In real-world applications, experiments are often contaminated by measurement noise, while computer simulations may be polluted by numerical noise. This noise introduces a non-deterministic element, rendering the response of a model or experiment a random variable, even when the input parameters are fixed. This non-deterministic model behaviour is typical of stochastic simulators. These simulators are pertinent when latent sources of uncertainty impact a system, resulting in the response being a random variable conditioned on the input parameters. Stochastic simulators can effectively capture the noisy nature of both high- and lower-fidelity models. To alleviate the cost of repeatedly evaluating stochastic simulators, different methods exist to emulate their response. Such approaches can be statistical, replication-, or spectral expansions-based. This work explores the synergy between MFSMs and stochastic simulators, paving the way for the development of multi-fidelity stochastic emulators.

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MS99

Construction and Performance of Polynomial Chaos Surrogates for Stochastic Processes

Mesoscopic modeling of surface chemistry bridges atomistic and continuum modeling of surface kinetics. Studying these models is crucial for understanding events relevant in surface catalysis such as localized coverage-dependent processes. Together, underlying stochasticity of such systems and uncertainty in chemical rates impact model predic-

tions and inflate the computational expense for obtaining converged estimates of the system state. Thus, UQ and global sensitivity analysis require construction of accurate spatiotemporal surrogates. Development of such surrogates is further challenged by the large number of input parameters and dimensionality of the system. Motivated by applications in surface kinetics, we develop a general methodology for constructing surrogate representations for high-dimensional stochastic fields. Resulting surrogates efficiently map uncertain rate parameters to random field quantities of interest associated with the surface reactions. Notably, each surrogate representation is in a joint space of *both* parametric uncertainty and intrinsic noise. We detail the construction and compare performance of multiple surrogates which differ primarily in their representation of intrinsic stochasticity. We demonstrate the technique on relevant surface reaction models and examine the sensitivity of the output quantities with respect to model parameters.

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MS99

Bayesian Model Updating for Frequency Domain Data Using Active Learning Based Sparse Bayesian Rational Polynomial Chaos Surrogate Model

Surrogate models enable the efficient propagation of uncertainties in computationally demanding models of physical systems. Our focus lies on linear structural dynamics problems, for which the system response can be described by the frequency response function. To this end, we employ a surrogate model that expresses the system frequency response as a rational function of two polynomial expansions in terms of the system parameters. Recently, a sparse Bayesian learning approach for rational approximation was proposed in which only the polynomial terms that significantly contribute to the predictability of the surrogate are retained. The proposed approach is based on global, static experimental designs. However, it can be beneficial to resort to active learning approaches for specific applications, such as optimization or Bayesian updating. In active learning, the experimental design is adaptively enriched during the training process based on a so-called acquisition function. In this contribution, we assess simulation- and approximation-based approaches to active learning using rational surrogate models. We specifically focus on Bayesian updating problems in which we are interested in estimating the mode of the posterior distribution of a set of system parameters based on measured frequency response data and demonstrate the applicability of the presented methods on different dynamic models.

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MS99

A Generalized Physics-informed Polynomial Chaos Framework for Surrogate Modeling and Uncertainty Quantification

Polynomial chaos expansion (PCE) is a widely adopted surrogate modeling method primarily employed in uncertainty quantification (UQ) and, more recently, in the field of machine learning (ML). PCE surrogate models are trained using a limited number of deterministic simulations from computationally expensive models to yield pointwise predictions within the design space. However, ensuring an accurate approximation of the underlying model may require a considerable number of computationally expensive simulations, which is often challenging with physics-based models. To reduce the training data requirement for precise predictions, we can supplement the limited data with the known physics of the model, thereby improving the accuracy and computational efficiency. This work presents a novel generalized physics-informed PCE framework for incorporating various types of known physical constraints, such as initial and boundary conditions, governing partial differential equations, and inequality-type constraints (e.g., monotonicity, convexity, non-negativity). We demonstrate that the proposed method shows a high level of accuracy while significantly decreasing the need for expensive simulations run for training. Furthermore, the predictions adhere to the physical laws throughout the entire design space, making it ideal for UQ and ML applications involving physical models.

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MS100

A Deep Learning Approach to Thermospheric Density Modeling with Uncertainty Quantification for Enhanced Orbit Prediction

Conjunction analysis and collision avoidance in space operations have become increasingly vital due to the growing population of space objects (SOs). Notably, 57% of these objects are situated in the low Earth orbit (LEO) and are heavily influenced by Earth's upper atmosphere, making precise orbit determination and prediction contingent upon accurate drag force estimations originating from this region. However, modeling and forecasting this drag force pose significant challenges, primarily due to the complex and ever-changing nature of the ionosphere-thermosphere system. Traditionally, thermospheric mass density is esti-

mated using either empirical models or physics-based models. Empirical models offer rapid predictions but exhibit limited accuracy. Conversely, physics-based models deliver superior forecasting capabilities but demand substantial computational resources. In our research, we introduce a dynamic data-driven reduced-order thermospheric density model that combines the predictive strengths of physics-based models with the computational efficiency of empirical models. It achieves this by projecting the high-dimensional space characterizing thermospheric mass density onto a lower-dimensional space. Consequently, this dynamic data-driven model enhances our ability to quantify uncertainties associated with the propagated SOs, contributing to safer and more efficient space operations.

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MS100

Cislunar Uncertainty Propagation and Bayesian Inference

Tracking algorithms provide a fundamental element of space domain awareness by producing up-to-date information on the state (e.g., position and velocity) of objects of interest. One way to obviate the need for advanced tracking algorithms is to attempt to overcome any lack of knowledge through the deployment and acquisition of an ever-increasing amount of information. The need for advancements in tracking algorithms for natural and artificial space objects is greatly exacerbated by the growing pressure being placed on the space domain by the presence of large satellite constellations and the growing interest in the cislunar orbital regime. Previous work in this domain has focused primarily on the propagation of uncertainty in the presence of nonlinear dynamics, and it has been shown that Gaussian mixture representations are better able to approximate the underlying probability distribution for space object tracking. This work leverages these uncertainty propagation results and investigates corresponding approximate Bayesian inference for space object tracking in the cislunar regime using Gaussian mixture representations of uncertainty. The new method is demonstrated on illustrative problems, including examples relevant for cislunar space domain awareness. The new approach is shown to recover the existing methods for the case of linear measurements (which is unrealistic in the space environment) and to improve upon existing methods in the presence of nonlinear measurements.

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MS100

Nonlinear Filtering with Multi-Fidelity Polynomial Chaos

In stochastic systems with nonlinear dynamics and measurement models, state of the art linear filtering methods are often unable to provide consistent estimates. This has led to a proliferation of nonlinear uncertainty quantification (UQ) and filtering methods over the last few decades. Polynomial Chaos Expansion (PCEs), a subset of these methods, approximate higher moments of probability distributions by projecting a stochastic solution onto an orthogonal polynomial basis. PCEs are capable of modeling non-Gaussian uncertainty over sparse measurement sets and long propagation times and have been shown to be more efficient than sampling-based methods. Multi fidelity methods, where a low number of high-fidelity solutions can be used to correct a larger group of lower fidelity solutions, have also seen use in UQ to achieve balance between efficiency and accuracy. This work demonstrates a previously presented nonlinear filter using a PCE-based update with the addition of multi-fidelity methods to the propagation step. Because the intrusive polynomial chaos used in the filter also involves altering the equations of motion governing the system of interest through spectral projection, this work investigates the use of nonintrusive PCEs as a high-fidelity component to the lower fidelity intrusively propagated solution, thus increasing the accuracy of the propagation step in the filter while avoiding additional algorithmic complexity.

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MS100

Likelihood Scouting via Map Inversion For A Posterior-Sampled Particle Filter

An exploit of the Sequential Importance Sampling (SIS) algorithm using Differential Algebra (DA) techniques is derived to develop an efficient particle filter. The filter creates an original kind of particles, called scout particles, that bring information from the measurement noise onto the state prior probability density function. Thanks to the creation of high-order polynomial maps and their inversions, the scouting of the measurements helps the SIS algorithm identify the region of the prior more affected by the likelihood distribution. The result of the technique is two different versions of the proposed Scout Particle Filter (SPF), which identifies and delimits the region where the true posterior probability has high density in the SIS algorithm. Four different numerical applications show the benefits of the methodology both in terms of accuracy and efficiency, where the SPF is compared to other particle filters, with particular focus on target tracking and orbit determination problems.

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MS101

The Innovation Ecosystem of North-East of Italy: Challenges and Opportunities

We will introduce the Innovation Ecosystem of North-East of Italy with 9 thematic Spokes in 9 Universities nurturing

innovation and enhancing technology transfer with industry and society.

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MS101
Digital Twins and UQ: an Integration Perspective

UQ is playing a very important role in digital twins development since they deal with real data assimilated from several sources. A wider perspectives will be provided to integrate data, HPC (high performance computing), UQ, and ROM (Reduced order modelling) with example of applications.

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MS101
The North-East Innovation Ecosystem: the ambitious scientific mission

We will provide an overview about the scientific mission of the North-East Innovation Ecosystem within its territory and its complex, ambitious, as well as involving goals by focusing on the receipts enhancing the advances of science for industry and society thanks to emerging technologies.

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MS101
Digtal Twin of the Ocean: an European Mission

Spoke 8 of Innovation Ecosystem of North-East of Italy is also dedicated to the development of complex digital twins of the sea: this is a very ambitious goal where uncertainty quantification plays a crucial role together with other emerging disciplines.

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MS102
Neural Latent Dynamics Models

Solving differential problems using full order models (FOMs), like the finite element method, incurs prohibitively computational costs in real-time simulations and multi-query routines. Reduced order modeling aims at replacing FOMs with reduced order models (ROMs), that exhibit significantly reduced complexity while retaining the ability to capture the essential physical characteristics of the system. In this respect, the novel concept of the Latent Dynamics Problem (LDP) is introduced and the class of Latent Dynamics Models (LDMs), along with their specialized deep learning counterpart, Neural Latent Dynamics Models (NLDMs) is presented. NLDMs constitute a neural differential equations-based model architecture designed for continuous-time modeling. This architecture is embedded within a reduced order modeling framework, with the primary objective of capturing the latent, low-dimensional dynamics of high-dimensional dynamical systems. In a series of numerical experiments, the effectiveness of NLDMs in addressing challenging problems is demonstrated, particularly in the context of large-scale high-fidelity models governed by time-dependent parameterized PDEs. The results not only underscore the remarkable performance of NLDMs but also highlight their potential as a valuable tool for understanding and modeling complex dynamic systems.

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MS102
Hybrid Data-Driven Strategies for Parametric Reduced Order Modeling

The present contribution deals with parametric Reduced Order Models (ROMs) for turbulent flows, in the realm of Computational Fluid Dynamics. Typically, ROMs employ a limited number of basis functions to minimize the computational cost. However, when dealing with marginally-resolved modal regimes, this approach can lead to inaccuracies. To enhance the accuracy while maintaining a low computational effort, we combine ROMs with stabilization techniques. Our approach is based on Proper Orthogonal Decomposition (POD) and focuses on intrusive POD-Galerkin ROMs. In this framework, we combine physics-based and purely data-driven methods that are built using machine learning techniques. In particular, the physics-based approach integrates the turbulence modeling into the reduced system, whereas the purely data-driven approach is aimed to reintroduce the contribution of the discarded modes, following a Variational Multi-Scale logic. The innovation of this work consists in the application of the above-mentioned approaches to parametric turbulent test cases, where the need of creating a unique model for all parameter values increases the model complexity. Our findings demonstrate that these techniques yield significantly improved results compared to the original not stabilized ROM, enhancing both velocity and pressure approximations.

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MS102
PDE-Constrained Deep Kernel Learning for High Dimensional Problems

The task of modeling and numerically experimenting with high-dimensional partial differential equations (PDEs) has garnered significant attention. The key idea for this work centers on leveraging PDE information to construct deep

kernel architectures with facilitated uncertainty quantification. In particular, a probabilistic machine learning tool – *Deep Kernel Learning* (DKL) – is used to embed neural network structures into Gaussian processes. Our method incorporates governing PDEs into DKL and maps data into a low-dimensional feature space, which not only enhances the ease of regression but also extends PDE-constrained Gaussian processes with improved nonlinear expressivity. Numerical results show that such an integration promises enhanced robustness and versatility in surrogate modeling. Crucial technical aspects include the selection of appropriate network structures, optimal parameter initialization, and meticulous hyperparameter tuning. We propose tailored optimization settings to tackle the challenges in such a high-dimensional approximation task.

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MS103

Random Persistence Diagram Generator

We will present a random persistence diagram generator (RPDG) method that generates a sequence of random persistence diagrams from the ones produced by the data. RPDG is underpinned by a model based on pairwise interacting point processes and a reversible jump Markov chain Monte Carlo (RJ-MCMC) algorithm. A first example, which is based on a synthetic dataset, will demonstrate the efficacy of RPDG and provides a comparison with another method for sampling PDs. A second example will demonstrate the utility of RPDG to solve a materials science problem given a real dataset of small sample size.

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MS103

Intrinsic Models in Wasserstein Space with Applications to Molecular Dynamics

We study the problems of efficient modeling and representation learning for probability distributions in Wasserstein space. We consider a general barycentric coding model in which data are represented as Wasserstein-2 (W2) barycenters of a set of fixed reference measures. Leveraging the geometry of W2-space, we develop a tractable optimization program to learn the barycentric coordinates and provide a consistent statistical procedure for learning these coordinates when the measures are accessed only by i.i.d. samples. Our consistency results and algorithms exploit entropic regularization of the optimal transport problem and the statistical convergence of entropic optimal transport maps will be discussed. We also consider the problem of learning reference measures given observed data. Our regularized approach to dictionary learning in W2-space addresses core problems of ill-posedness and in practice learns interpretable dictionary elements and coefficients useful for downstream tasks. Applications of optimal transport to compression of molecular dynamics simulations will be considered.

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MS103

Generative Diffusion Learning for Parametric PDEs

We present a novel probabilistic formulation of the operator learning problem based on recently developed generative denoising diffusion probabilistic models (DDPM) in order to learn the input-to-output mapping between problem parameters and solutions of the PDE. To achieve this goal we modify DDPM to supervised learning in which the solution operator for the PDE is represented by a class of conditional distributions. The probabilistic formulation combined with DDPM allows for an automatic quantification of confidence intervals for the learned solutions.

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MS104

Efficient Sensitivity Analysis for Biomechanical Models with Correlated Inputs

In most variance-based sensitivity analysis (SA) approaches applied to biomechanical models, statistical independence of the model input is assumed. However, often the model inputs are correlated. This might alter the interpretation of the SA results, which may severely impact the guidance provided during model development and personalization. This study aimed to propose an efficient correlated global SA method by applying a surrogate model-based approach. Furthermore, this paper demonstrates how correlated SA should be interpreted and how the applied method can guide the modeler during model development and personalization. The proposed methodology was applied to a typical example of a pulse wave propagation model and resulted in accurate SA results that could be obtained at a theoretically 27000x lower computational cost compared to the correlated SA approach in which we do not use a surrogate model. Furthermore, our results demonstrate that input correlations can significantly affect SA results, which emphasizes the need to thoroughly investigate the effect of input correlations during model development. We conclude that our proposed surrogate-based SA approach allows modelers to efficiently perform correlated SA to complex biomechanical models and allows modelers to focus on input prioritization, input fixing and model reduction, or assessing the dependency structure between parameters.

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MS104

Methods for Domain Preservation in Stochastic Biological Systems

Many stochastic (partial) differential equations that arise in mathematical biology preserve positivity (eg concentrations should be positive) or solutions should lie in a certain domain (eg $[0, 1]$ for stocastic gating variables). The question then arises how to preserve these domains in a numerical simulation. We develop a numerical method based

on exponential integrators that naturally preserve such domains and discuss convergence and efficiency. This work is joint with Utku Erdogan.

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MS104

The Numerical Solution of Stochastic Neural Field Problems

We consider strong convergence of space-time discretizations of neural field equations with additive noise. Our methods are variants of exponential based methods in time and we examine projection and collocation methods in space. We introduce the neural field equations, some properties of solutions before we outline the proof of strong convergence. Numerically we compare the efficiency of methods. The study of these time integrators of stochastic neural fields is interesting in its own right, but is also an important stepping stone for addressing inverse problems.

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MS104

Inverse Uncertainty Quantification and Forward Uncertainty Propagation in Reaction Network Models

Signalling pathways within neurons can be described via reaction networks. Different approaches can be used to model these biological systems: among others, ODE models describe the time evolution of concentrations of reaction compounds, while stochastic models allow us to simulate the number of molecules in the system. In both types of models, reaction rate constants are treated as model parameters. Using experimental data we perform inverse uncertainty quantification on the model parameters in the Bayesian framework. In particular, we use methods from the class of Markov chain Monte Carlo methods to approximate the parameter posterior distribution. We consider both likelihood-based (SMMALA) and likelihood-free (ABC-MCMC) methods. The uncertainty in the parameters is propagated to predictions and global sensitivity analysis can be performed based on the posterior distribution. We developed an R package, uqsa, that performs many of these tasks. We describe uqsa and show uncertainty quantification results on models and data from neuroscience.

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MS105

Combination of Gaussian Process Models with Random Length-Scales for High-Dimensional Bayesian Optimization

Gaussian Processes (GPs) are commonly used as surrogate models of expensive computer codes in design optimization where Bayesian approaches, such as efficient global optimization (EGO), are employed to speed-up the optimization process. These methods have been successfully applied to many real-world applications in low dimensions (less than 30). However, in higher dimensions, building an accurate GP surrogate model is met with various setbacks. The optimization of the covariance length-scale hyperparameters which is typically performed by maximizing the log-likelihood of the model often fails to provide correct values. In this talk, we present a new method for high-dimensional GP models which bypasses the length-scales optimization by combining sub-models with random length-scales. We obtain a closed-form expression of the combination and we describe an approach to sample suitable length-scales using a criterion based on the entropy of the correlations. Finally, we present a way to obtain the prediction variance of the combination and we apply our combined model to high-dimensional EGO. We show that the classical GP approach using maximum likelihood estimation fails to properly optimize the length-scale hyperparameters and that our method successfully builds more accurate surrogate models for EGO, thus reducing the number of computer code evaluations to obtain optimal designs.

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MS105

Comparing Scale Parameter Estimators for Gaussian Process Regression: Cross Validation and Maximum Likelihood

Gaussian process (GP) regression is a Bayesian nonparametric method for regression and interpolation, offering a principled way of quantifying the uncertainties of predicted function values. For the quantified uncertainties to be well-calibrated, however, the covariance kernel of the GP prior has to be carefully selected. In this work, we theoretically compare two methods for choosing the kernel in GP regression: cross-validation and maximum likelihood estimation. Focusing on the scale-parameter estimation of a Brownian motion kernel in the noiseless setting, we prove that cross-validation can yield asymptotically well-calibrated credible intervals for a broader class of ground-truth functions than maximum likelihood estimation, suggesting an advantage of the former over the latter.

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MS105

Kernel with Sinkhorn Optimal Transport

Machine learning tasks, and arises in a large range of applications. Among various existing approaches to tackle this problem, kernel methods have become a method of choice. Indeed, kernel distribution regression is both computationally favorable, and supported by a recent learning theory. This theory also tackles the two-stage sampling setting, where only samples from the input distributions are available. In this paper, we improve the learning theory of kernel distribution regression. We address kernels based on Hilbertian embeddings, that encompass most, if not all, of the existing approaches. We introduce the novel near-unbiased condition on the Hilbertian embeddings, that enables us to provide new error bounds on the effect of the two-stage sampling, thanks to a new analysis and , we strictly improve the existing convergence rates for these kernels.

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MS106

Sampling Criteria for Excursion Set Estimation on Multi-Output Models

Many industrial issues are related to excursion set estimation problems, under the form of estimation of a set of feasible black box model input values, corresponding for instance to feasible optimal design schemes. The set we aim to estimate, called excursion set, is then defined as the set of model input values satisfying a constraint on a model output, for example to remain below a fixed threshold. An effective way to solve this problem is to model the costly black-box function of interest as a realization of a Gaussian process (GP). This surrogate model is learned thanks to a sequential Design of Experiments, whose points are chosen accordingly to the optimization of an acquisition criterion. In this work, we focus on black-box costly models with vectorial output. Our aim is to estimate all partial excursion sets for each output. We propose an extension of the Bichon criterion, the classic criterion for excursion set estimation. The proposed extension is based on the minimum of the distances between each component of the GP and the corresponding threshold. It requires calculation of orthants probabilities of multivariate normal distributions.

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MS106

Using Gaussian Mixture Models to Solve Inverse Problems with Full Bayesian UQ

Atmospheric remote sensing (e.g. measuring carbon dioxide or methane) requires solving a non-Gaussian inverse problem thousands of times per second. Standard Bayesian inference algorithms which rely on repeated evaluation of a likelihood function are computationally unnecessarily expensive, which proves to be a bottleneck in operational processing. Furthermore, current algorithms rely on Gaussian approximations and fail to accommodate forward modeling error. We propose a new method to sidestep these problems by modeling the joint distribution of the observations and outputs as a Gaussian Mixture that we then condition by measured data. Once trained, the GMI can be conditioned on observations in negligible computational time, while yielding a high quality non-Gaussian representation of the true posterior distribution. Our method can also accommodate a range of prior and measurement error models, going beyond the usual Gaussian approximation. We demonstrate the effectiveness of the method in computational toy inverse problems and with NASAs Orbiting Carbon Observatory 2 Satellites carbon dioxide inverse problem. Our results are compared against posterior distributions obtained via MCMC, showing remarkable agreement with negligible computational cost.

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MS106

Uncertainty Propagation and Sensitivity Estimation via Temporal Normalizing Flows

Dynamical systems play a vital role in modeling complex temporal and spatio-temporal phenomena with applications spanning climate, finance, biology, and geophysics. These systems are often characterized by parameter-

dependent differential equations that describe the evolution of state variables over time and space. We extend adjoint-based a posteriori analysis for differential operators of generic dynamical systems acting on states to the Liouville operator acting on probability densities of the states resulting in theoretically rigorous estimates of sensitivity and error for a broad class of computed QoI. To make these estimates computationally tractable, normalizing flows exploiting the hyperbolic nature of the Liouville equation (which is also used in Neural ODEs) are utilized to construct a spatio-temporal density estimator via a loss function defined from a combination of Kullback-Leibler (KL) divergence and a Physics informed Loss function. We also derive computable error estimates when utilizing an estimator of the PDF in computing the QoIs. We consider a Neural ODE and compute sensitivities of QoIs to the network parameters.

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MS106

Adaptively Calibrated Optimization-Based Confidence Intervals for Inverse Problem Uncertainty Quantification

We address the need for functional uncertainty quantification for inverse problems where it is possible to evaluate a forward model, the observation noise distribution is known, and there are known parameter constraints. The strict bounds method of Burrus/Rust/OLeary/Tenorio/Stark neatly formulates confidence interval computation as two endpoint optimizations, where the optimization constraints can be set to achieve different types of interval calibration while seamlessly incorporating parameter constraints. Although there is a clear constraint setting to obtain simultaneously covering intervals, one-at-a-time intervals with coverage for a single functional have been elusive. We propose a new simulation-based quantile regression method for setting the endpoint optimization constraints to guarantee one-at-a-time coverage. This method is built upon viewing the strict bounds intervals as the inversion of a particular likelihood ratio test and operates by sampling from log-likelihood ratio test statistic distributions under a particular collection of null hypotheses. This collection depends on the observed data, rendering the optimization constraints (and therefore the confidence interval length) adaptive to the underlying true parameter.

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MS107

Detection of Model-form Error Through Information Field Theory

We derive properties of information field theory (IFT) as applied to inverse problems. The results here can be extended to methodologies which can be seen as limiting cases of IFT, such as Gaussian process regression and physics-informed machine learning. We first define the concept of a well-posed inverse problem within the context of IFT, and pose a few useful theorems for conditions in which an inverse problem becomes well-posed. Using the Gaussian random field interpretation of IFT, we show how identifying parameters of a covariance kernel becomes a well-posed inverse problem under certain conditions. An expression for the Hessian of the inverse problem log posterior is derived to construct the results. A specific focus is placed on the inverse problem of detecting model-form error. We provide an example where the physics are assumed to be the Poisson equation and prove conditions for which identifying model-form error in this case becomes a well-posed inverse problem under IFT.

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MS107

Information Field Theory: Concepts and Applications

Inferring a physical field from data is an ill posed problem, as the finite data can not alone constrain the infinite number of degrees of freedom of a function over continuous space. Domain knowledge has to regularize the set of possible solutions, however, usually significant uncertainties remain and need to be quantified. This can be done via information field theory (IFT), which is a mathematical formulation of probabilistic signal field inference. Here, the basic concepts of IFT and its numerical implementation are introduced and its application to astrophysical datasets are shown.

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MS108

Sparsifying Dimensionality Reduction of PDE Solution Data with Bregman Learning

Classical model reduction techniques project the governing equations onto a linear subspace of the original state space. More recent data-driven techniques use neural networks to enable nonlinear projections. Whilst those approaches are not limited by the Kolgomorov n-width, they lack the ability to guarantee a physically meaningful representation of PDE-generated data and may overestimate

the latent dimensionality. To overcome these, we propose a multistep algorithm that induces sparsity in the encoder-decoder networks for an effective compression of the latent space. In the first step, we train a sparsely initialized network using linearized Bregman iterations. In the second step, we further compress the latent space dimensionality by POD. Afterwards, we use a bias propagation technique to reduce the network density even further. We apply this algorithm to three representative PDE models: 1D diffusion, 1D advection, and 2D reaction-diffusion. Compared to conventional training methods like Adam, our method achieves similar accuracy with 30% less parameters and a significantly smaller latent space.

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MS108

Predictive Digital Twins for Optimized Management and Maintenance of Civil Structures

The digital twin concept represents an appealing opportunity to enable condition-based and predictive maintenance approaches for civil structures. This paradigm shift holds the potential for reduced lifecycle costs, enhanced system safety, and improved system availability. In this talk, we introduce a digital twin framework designed to facilitate personalized monitoring, management and maintenance programs for civil structures. The asset-twin coupled dynamical system and its evolution over time are encoded using a probabilistic graphical model. Specifically, the observations-to-decisions flow is modeled through a dynamic Bayesian network, allowing for the incorporation of uncertainties inherent to real-world conditions. Observational data are assimilated with deep learning models to provide real-time structural health diagnostics. This continually updates the digital twin state through sequential Bayesian inference. The updated digital state is then employed to forecast future damage growth, thereby informing optimal planning of maintenance and management actions within a dynamic decision-making framework. A preliminary offline phase involves the population of training datasets through a reduced-order numerical model and the computation of a health-dependent control policy. To illustrate the dynamic decision-making capabilities of health-aware digital twins, the strategy is assessed through two synthetic case studies involving a cantilever beam and a railway bridge.

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MS108

Deep Learning Enhanced Cost-Aware Multi-Fidelity Uncertainty Quantification of a Computational Model for Microcirculation

Forward uncertainty quantification (UQ) for partial differential equations is a many-query task that requires a significant number of model evaluations. We present in this work a deep learning enhanced multi-fidelity Monte Carlo (MFMC) method and an application to a 3D-1D computational model for microcirculation, with a focus on oxygen transfer in vascularized biological tissue. A deep learning enhanced non-intrusive projection-based reduced order model (ROM) is exploited as a surrogate of the high-fidelity full order model (FOM), that hinges upon finite-element approximations of the solution. The proposed approach adapts a developed MFMC method, minimizing the upper bound of the mean-squared errors of the estimator and providing an optimal balance between the offline training cost of the low-fidelity ROM with the online sampling costs and, given a computational budget time. The adopted low-fidelity ROM is built in a supervised learning framework, provided the optimal number of FOM training samples. Based on standard proper orthogonal decomposition (POD) approach and leveraging Mesh-Informed Neural Networks, it combines together a neural network approximating the POD coefficients and a closure model acting as fine-scale corrector for the local structures not captured by the former. We exploit the relevant ROM speed-up to accelerate the estimation of statistics of oxygen-related and radiotherapy quantities of interest, performing a robust and reliable UQ analysis.

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MS108

Deep Generative Modeling for Data-Driven Identification of Noisy, Non-Stationary Dynamical Systems

An important challenge in many fields of science and engineering is making sense of a deluge of time-dependent measurement data by recovering the governing equations in the form of ordinary or partial differential equations. We are interested in finding interpretable, parsimonious models in the form of closed form differential equations for nonlinear, noisy, and non-stationary dynamical systems. To this end, we propose a machine learning method that performs system identification in such systems. An array of methods so far have addressed noisy and limited data; however, the problem of non-stationarity, when parameters describing the differential equations have explicit time dependence, has received considerably less attention. In this work, we combine a framework for data-driven dis-

covery of stochastic differential equations using hypernetworks and the SINDy (sparse identification of nonlinear dynamics) method with a recurrent network module to identify the parametric time dependencies. The result is a novel approach *dynamic HyperSINDy* to system identification of stochastic, non-stationary dynamical systems. We test our method on synthetic data using simple canonical systems, including non-linear oscillators with underlying time-dependent parameters, and the chaotic Lorenz system. The aim is to extend dynamic HyperSINDy to a wide range of problems, specifically on dynamic systems where complex parametric time dependencies are expected.

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MS109

A Flexible Transport Map Approach for Bayesian Optimal Experimental Design

We present an approach for approximating expected utility functions arising in Bayesian optimal experimental design (BOED) problems characterized by intractable posterior densities. Our method, which is based on transportation of measures, is applicable to a wide range of BOED problems and can accommodate various optimality criteria, prior distributions and noise models. We explain the key ideas of our approach and comment on extensions to adaptive or sequential optimal design. The effectiveness of our approach is illustrated with a few numerical examples.

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MS109

New Aspects on a Convex Approach to Optimum Design of Experiments with Correlated Observations

The method of virtual noise has been propagated to solve optimum experimental design problems for models with correlated observations. We show that it is compatible with other reecently suggested approaches and present some improvements on a range of examples.

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MS109

An Ensemble-Based Approach to Optimal Experimental Design for Large-Scale Nonlinear Inverse Problems

Ensemble Kalman methods form a set of derivative-free algorithms widely used for approximating the solutions to statistical inverse problems with complex forward models, in areas including climate modelling, engineering and geophysics. In this work, we study the incorporation of ensemble Kalman methods into the optimal experimental design (OED) framework. In particular, these methods open the door to the use of OED with simulators for which derivatives are unavailable, and with measures of uncertainty other than local covariance information. We demonstrate the application of our proposed methodology to large-scale inverse problems arising in subsurface flow and geothermal reservoir engineering.

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MS110

Recent Enhancements of the Nonparametric Probabilistic Method for Uncertainty Quantification

The nonparametric probabilistic method (NPM) is a computational framework that enables the modeling and quantification of model-form uncertainty by fusing sensor data and lower-dimensional physics-based computational models. It leverages projection-based model order reduction to generate a computationally tractable data-enriched stochastic model; then to deliver in real-time numerical predictions in the form of confidence intervals containing the true values of the unknown quantities of interest (QoIs), within a specified confidence level. Starting from a deterministic high-dimensional model, NPM constructs first a deterministic reduced-order basis. Then, it randomizes it on a compact Stiefel manifold using a small number of hyperparameters, to build a stochastic projection-based reduced-order model (SPROM). Using this model, NPM identifies next the hyperparameters by formulating and solving an inverse statistical problem founded in data. Specifically, NPM seeks to minimize the distance between the predicted mean and fluctuations of the family of QoIs it predicts using the SPROM, and their counterparts it extracts from sensor data. The stochastic and non-convex nature of the optimization problem makes it robust and optimal solution challenging, particularly in the context of scarce sensor data. This main issue is addressed in this talk in the form of enhancements to the formulation of the low-dimensional inverse statistical problem and its optimization framework.

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MS110

Robust Bayesian Optimal Experimental Design for Misspecified Linear and Nonlinear Models

Bayesian optimal experimental design (BOED) is increasingly used to close the loop in uncertainty quantification. Choosing the optimal way to gather data or other information helps scientists and engineers work within limit budgets to achieve their uncertainty goals. However, as with all methods, understanding the impact of assumptions or discrepancy is critical. In some cases this is particularly important for BOED because it guides the way data is gathered, which can lead to BOED not sampling data that could falsify assumptions. In this talk we discuss two information criteria for linear and non-linear BOED problems that incorporate notions of model discrepancy. These criteria are intended to augment traditional BOED based on Expected Information Gain by defining a trade off in robustness vs performance of the experimental design. The first criteria is the Expected Generalized Information Gain which measures a notion of how poor inference using an incorrect model is expected to perform compared to the true model. The second criteria is the Expected Discriminatory Information which defines how well the expected data from the experiment could be used to invalidate a model. Beyond discussing these criteria in general, we will discuss the computational methods required to estimate them for non-linear models.

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MS110

Correcting for Error in Reduced-Order Modeling Using Experimental Partial Observations and Bayesian System ID

In the traditional reduced-order modeling setting, full-field data collected from simulation of a full-order model (FOM) are used to estimate a low-dimensional approximation of the FOM. In practice, however, FOMs are almost always inaccurate, uncertain, or partially unknown, which limits the level of accuracy that can be achieved by a reduced-order model (ROM). Data-driven estimation techniques can improve the FOM accuracy but are challenging for two main reasons. The first is that estimation is computationally burdensome since it usually involves many forward evaluations of an expensive FOM. The second is that the system of interest can often only be measured through noisy partial observations that introduce high uncertainty into the estimation problem. In this work, we propose a method for learning reduced-order closure models that is capable of addressing both of these challenges. Firstly, evaluation of the FOM is avoided by performing estimation in the reduced-dimensional space such that only forward evaluations of the ROM are needed. Secondly, we use a Bayesian learning framework that addresses the model uncertainty of the ROM and the measurement uncertainty of the noisy partial observations to deliver robust estimation under uncertainty. The merits of this method will be demonstrated on numerical examples of systems of partial differential equations.

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MS110

Model Discrepancy for Laminar Hypersonic Flow

Despite continuing advances in statistical inversion and modeling, model inadequacy due to model form error remains a concern in all areas of mathematical modeling. The Bayesian paradigm naturally integrates uncertainties from both experimental data and model formulation, including initial or boundary conditions, model form, and parameter and numerical approximation. While model improvement is an enterprise that is continuously enabled by the availability of cost-effective high-performance computing infrastructure, model error is unavoidable in many situation. This problem is attributed to the incomplete understanding of the underlying physics, likely in addition to large and poorly characterized uncertainties in calibration and validation data. Introducing a model discrepancy term into the Bayesian framework can improve the predictive power of a given model and, arguably, the transferability of physical parameters. Much like physical models, calibrating a discrepancy model requires careful consideration regarding formulation, parameter estimation, and uncertainty quantification, each of which is often problem-specific. Several methodologies are presented, with an application to hypersonic re-entry experimental data. *SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

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MS111

Efficient Data-Driven Modeling of PDEs

The flow map learning framework is capable of learning the evolution of unknown ordinary and partial differential equations systems given access to observations of solution vectors. For partially-observed systems, a memory period is required to learn the reduced system. If the solution vector is high-dimensional and a long memory period is required, the model input can become burdensome. E.g., if the solution vector is observed on a 50x50 grid and needs 20 memory steps, then the input will be of dimension 50,000. For neural network based models, a high-dimensional input greatly increases the number of hidden parameters in the model regardless of the complexity of the function being modeled. This in turn requires more data to appropriately learn the hidden parameters without overfitting. In contrast, real world problems frequently require modeling with limited data. Therefore, it is desirable to be able to model complex systems with fewer parameters. This talk will discuss several new approaches to this issue.

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MS111

Characterizing Data-Driven Surrogate Models for Wildfires

Each year, wildfires cause injury, death, and billions of USD in damages. Forecasting future fire behavior and impacts with state-of-the-art codes is computationally challenging, and this becomes intractable over large spatial and time scales. However, outer-loop problems (e.g., fuel-content inversion) require repeated evaluations of the underlying physics. In this context, therefore, one needs a computationally inexpensive but still reasonably accurate *surrogate model*. There has been much recent methodological work on surrogate models. However, the comparative strengths and weaknesses of these various methods are not well understood for wildfire simulation. In this talk, we will survey several contemporary surrogate models and apply them to wildfires, with a focus on the outer-loop problems of inversion and forecasting. Specifically, we will characterize the behavior of surrogates through the traits of robustness, scalability, and efficiency.

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Deep Learning for Model Correction

Despite many recent advances and new deep learning technologies, training of the Deep Neural Networks (DNNs) for modeling of unknown systems generally requires large amounts of high-fidelity training data. Such large quantities of data may not be available, hence it is of importance to develop methodologies that can accurately correct imperfect prior models given scarce amounts of high-fidelity data. Hence, utilizing DNNs and transfer learning, we present a model correcting framework and demonstrate its effectiveness on several numerical examples.

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MS112

Progressive Multi-fidelity Surrogate Modeling

Highly accurate datasets are often expensive and time-consuming to acquire, posing a significant challenge for applications that require precise evaluations across multiple scenarios and in real-time. Conversely, less expensive, low-fidelity data can be computed more effortlessly and encompass a broader range of scenarios. Leveraging multi-fidelity information can improve the prediction capabilities of surrogates. However, in practice, data may come from various sources and at different times, further complicating the modeling process. To address these challenges, we introduce a progressive multi-fidelity surrogate model that sequentially incorporates diverse data types using tailored encoders. Multi-fidelity regression from the encoded inputs to the target quantities of interest is performed using neural networks. Input information progressively flows from lower to higher fidelity levels through two sets of connections: concatenations among all the encoded inputs and additive connections among the final outputs. This dual connection system enables the exploitation of correlations among different datasets while avoiding catastrophic forgetting as new input data are integrated into the model. As a result, this data-driven method automatically adapts predictions based on available inputs, achieves high accuracy, and generalizes across time and parameters.

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MS112

Multilevel Active Subspaces for High Dimensional Function Approximation

The active subspaces (AS) method is a widely used technique for identifying the most influential directions in high-dimensional input spaces that affect the output of a computational model. However, the standard AS algorithm requires a large number of gradient evaluations (samples) of the input output map to achieve quasi-optimal reconstruction of the active subspace, which can lead to a significant computational cost if the samples include numerical discretization errors which have to be kept sufficiently small. To address this issue, we propose a multilevel version of the active subspaces method (MLAS) that utilizes samples computed with different accuracies, which are often available in scientific computing models. The MLAS method yields different active subspaces for the model outputs across accuracy levels, which can match the accuracy of single-level active subspace with reduced computational cost, making it suitable for downstream tasks such as function approximation. We demonstrate the practical viability of the MLAS method through numerical experiments based on random partial differential equations (PDEs) simulations.

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MS112

Multifidelity Estimators for Non-Deterministic Models

Multifidelity Uncertainty Quantification (MFUQ) allows for the reduction of the computational cost of uncertainty propagation for high-fidelity applications by fusing information from models with varying cost and accuracy. The efficiency of such methods is tied to the correlations that exist amongst the quantities of interest obtained from the various models. Most efforts in this area have focused on deterministic models where repeated evaluations for the same inputs produce the same output. In contrast, a non-deterministic model's response will vary even when evaluated for the same inputs due to an intrinsic and uncontrollable source of variability. This variability manifests as noise in the model's statistics, impacting the correlations and, therefore, the performance of MFUQ techniques. Since non-deterministic models appear in applications like turbulent flow simulations, particle-in-cell methods for plasmas, modeling of material microstructures, and radiation transport, developing efficient UQ strategies for this class of models is needed. Herein, we demonstrate how noise due to non-determinism has a non-trivial effect on the statistics which impact the effectiveness of existing MFUQ techniques. The Approximate Control Variate framework [Gorodetsky, 2020] is extended to incorporate non-deterministic model sets and used to analyze popular multifidelity strategies applied to such models. Various numerical and theoretical results highlight unique issues which arise.

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MS112

An MFNets Approach with Basis Adaptation for Efficient Data-Driven Surrogate Modeling

The accurate construction of surrogates with reduced amounts of data is a central problem in scientific computing applications like optimization and uncertainty quantification. In this work we extend the Multifidelity Networks (MFNets) approach introduced in [1]. MFNets arranges multiple low-fidelity models (of varying cost/accuracy) into a Directed Acyclic Graph to encode the models dependencies. Our extension consists in the integration of the basis adaptation for the polynomial chaos expansions introduced for the representation of each model/node. The use of basis adaptation aims at strengthening correlations among models and reducing the nodes dimensionality, which in turn reduces the size of the sought-after parameters. This latter aspect is paramount for lowering the data requirements of the method. Moreover, we will show that the enhanced correlation among models also decreases the dependence of the method on the graph, thus enhancing the generality of MFNets by extending its range of applicability to problems characterized by a weaker model correlation. We will discuss the method on an array of test problems, including the analysis of the dynamics of a finite element spent nuclear fuel assembly. [1] A. Gorodetsky, et al., Mfnets: data efficient all-at-once learning of multifidelity surrogates as directed networks of information sources, Computational Mechanics 68 (2021) 741758. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

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MS113

Discrete-Time Filtering Problem: Reconciling Deterministic and Stochastic Frameworks

For nonlinear dynamics, the optimal filtering developed in the framework of deterministic control theory leads to the so-called Mortensen estimator. It is well known that this estimator can be interpreted as a small noise asymptotic limit of a stochastic filtering problem for a continuous-time formulation. Here we propose to revisit the formulation of a Mortensen estimator in the context of discrete-time dynamics and show how such an estimator can also be interpreted as a small noise asymptotic limit of a stochastic filtering problem. These results pave the way for unifying deterministic and stochastic approaches and reconciling Bayesian filtering and optimal control for observation theory while shedding new light on approximated optimal control for nonlinear systems, such as the Extended Kalman Filter approach.

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MS113

Deterministic Particle Approximations for Optimal Stochastic Control

We discuss optimal control for stochastic differential equations of the form

$$dX_t = [f(X_t) + u(X_t, t)]\, dt + \sigma dW_t$$

for $X_t \in R^D$ and and scalar diffusion $\sigma \in R$. The goal is to minimise the cost functional

$$C[u] = E_u \left\{ \int_0^T \left(\frac{1}{2\sigma^2} \|u(X_t, t)\|^2 + U(x) \right) dt + v(X_T) \right\}$$

with respect to the feedback control function $u(x, t)$. The expectation is over paths of the controlled process. The nonlinear Hamilton–Jacobi–Bellmann equation for this finite horizon problems can be transformed into a *linear* backward PDE, see e.g. [H. J. Kappen, Linear theory for control of nonlinear stochastic systems. Physical review letters 95, 200201 (2005)]. The solution of this PDE can be further represented as the ratio of two densities which fulfil a forward filtering equation and a Fokker-Planck equation, respectively. Representing the densities by particles we derive deterministic particle flows which in the mean field limit converge to the corresponding PDEs. The work is an extension of [D. Maoutsa and M. Opper, Deterministic particle flows for constraining stochastic nonlinear systems. Phys. Rev. Research 4, 043035 (2022)] and [D. Maoutsa, S. Reich and M. Opper, Interacting particle solutions of Fokker–Planck equations through gradient-log-density estimation, Entropy 22, 802 (2020)].

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MS113

Bayesian Inference and Global Sensitivity Analysis for Ambient Solar Wind Prediction

The ambient solar wind plays a significant role in propagating interplanetary coronal mass ejections and is an essential driver of space-weather geomagnetic storms. A computationally efficient and widely used method to predict the ambient solar wind radial velocity near Earth involves coupling three models in different spatial regions: Potential Field Source Surface, Wang-Sheeley-Arge, and Heliospheric Upwind eXtrapolation. The model chain has 11 uncertain parameters that are mainly non-physical due to empirical relations and simplified physics assumptions. We, therefore, propose a comprehensive uncertainty quantification (UQ) framework that can successfully quantify and reduce parametric uncertainties in the model chain. The UQ framework utilizes variance-based global sensitivity analysis followed by Bayesian inference via Markov chain Monte Carlo to learn the posterior densities of the most influential parameters. The ensemble predictions generated from the learned posterior densities significantly reduce the uncertainty in solar wind velocity predictions near Earth.

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MS113

A Nonparametric Statistical Perspective on ODE-based Distribution Learning

Ordinary differential equations (ODEs), via their induced flow maps, provide a powerful framework to parameterize invertible transformations for representing complex probability distributions. While such models have achieved enormous success in machine learning, little is known about their statistical properties. This work establishes the first general nonparametric statistical convergence analysis for distribution learning via ODE models trained through likelihood maximization. We first prove a convergence theorem applicable to *arbitrary* velocity field classes $\mathcal{F}$ satisfying certain simple boundary constraints. This general result captures the trade-off between the approximation error and complexity of the ODE model. We show that the latter can be quantified via the C^1-metric entropy of the class $\mathcal{F}$. We then apply this general framework to the setting of C^k-smooth target densities, and establish nearly minimax-optimal convergence rates for two relevant velocity field classes $\mathcal{F}$: C^k functions and neural networks. The latter is the practically important case of neural ODEs. Our results also provide insight on how the choice of velocity field class, and the dependence of this choice on sample size n (e.g., the scaling of neural network classes), impacts statistical performance. We also discuss extensions of this theory to flow-matching methods and related alternative training methods for ODE models.

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MS114

Stochastic Asymptotic-preserving Bi-fidelity Method for Multiscale Spread of Epidemics Under Uncertainty

Addressing data uncertainty is a key challenge in epidemiological modeling. To create realistic scenarios of infection spread and devise effective control measures, it is crucial to have effective techniques that can measure the impact of random inputs on model outcomes. In this study, we propose a bi-fidelity approach to quantify uncertainty in epidemic models with spatial dependencies. This approach involves employing a high-fidelity model on a limited number of carefully chosen samples, guided by numerous evaluations of a low-fidelity model, ensuring both computational efficiency and accuracy [Liu, Pareschi, Zhu, J. Comput. Phys. 2022]. Specifically, we focus on a class of multiscale kinetic transport models as high-fidelity reference [Bertaglia, Liu, Pareschi, Zhu, Netw. Heterog.

Media 2022] and employ simpler discrete-velocity kinetic models for low-fidelity evaluations [Bertaglia, Pareschi, ESAIM: Math. Model. Numer. Anal. 2021]. Both model classes exhibit similar diffusive behaviors and are numerically solved using methods able to preserve their asymptotic limit, allowing to obtain stochastic asymptotic-preserving techniques. A series of numerical experiments demonstrates the soundness of the proposed approach.

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MS114

Single-Ensemble Multilevel Monte Carlo for Interacting Particle Methods

Interacting-particle methods have found applications in domains such as filtering, optimization and posterior sampling. These parallelizable and often gradient-free algorithms use an ensemble of particles that evolve in time, based on the combination of well-chosen dynamics and interaction between the particles. For computationally expensive dynamics for example Bayesian inversion with an expensive forward model, or optimization of an expensive objective function the cost of attaining a high accuracy quickly becomes prohibitive. We exploit a hierarchy of approximations to this forward model and apply multilevel Monte Carlo (MLMC) techniques, improving the asymptotic cost-to-error relation. More specifically, we use MLMC at each time step to estimate the interaction term within a single, globally-coupled ensemble. Numerical experiments corroborate our analysis of the improved asymptotic cost-to-error rate.

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MS114

Adaptive Parareal Algorithms and Application to the Simulation of Atomistic Defects

In this talk, we consider parareal algorithms in the context of molecular dynamics simulations. The parareal algorithm, originally proposed two decades ago, efficiently solves evolution problems by using parallel-in-time computations. It is based on a decomposition of the time interval into subintervals and makes use of a predictor-corrector strategy. It first uses a coarse, inexpensive solver to quickly step through the whole time domain, and next refines this approximate solution by using an accurate fine solver which is applied concurrently, in parallel, over each time subinterval. The prediction-correction process is repeated until convergence is reached. Although the parareal algorithm, in its original formulation, always converges, it suffers from various limitations in the context of molecular dynamics. In particular, it is observed that the algorithm does not provide any computational gain (in terms of wall-clock time compared to a standard sequential integration) in the limit of increasingly long time-horizons. This numerical observation is backed up with theoretical discussions. We introduce here a modified version of the parareal algorithm where the algorithm adaptively divides the entire time-horizon into smaller time slabs. We numerically show, on several test cases, that the adaptive algorithm overcomes the various limitations of the standard parareal algorithm, thereby allowing for significantly improved gains.

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MS115

Online Smoothing for Diffusion Processes Observed with Noise

We introduce a methodology for online estimation of smoothing expectations for a class of additive functionals, in the context of a rich family of diffusion processes (that may include jumps) observed at discrete-time instances. We overcome the unavailability of the transition density of the underlying SDE by working on the augmented pathspace. The new method can be applied, for instance, to carry out online parameter inference for the designated class of models. Algorithms defined on the infinite-dimensional pathspace have been developed the last years mainly in the context of MCMC techniques. There, the main benefit is the achievement of mesh-free mixing times for the practical time-discretised algorithm used on a PC. Our own methodology sets up the framework for infinite-dimensional online filtering an important positive practical consequence is the construct of estimates with variance that does not increase with decreasing mesh-size. Besides regularity conditions, our method is, in principle, applicable under the weak assumption relatively to restrictive conditions often required in the MCMC or filtering literature of methods defined on pathspace that the SDE covariance matrix is invertible.

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MS115

Information Gamma Calculus: Convexity Analysis for Stochastic Differential Equations

We study the Lyapunov convergence analysis for degenerate and non-reversible stochastic differential equations (SDEs). We apply the Lyapunov method to the Fokker-Planck equation, in which the Lyapunov functional is chosen as a weighted relative Fisher information functional. We derive a structure condition and formulate the Lyapunov constant explicitly. Given the positive Lypapunov constant, we prove the exponential convergence result for the probability density function towards its invariant distribution in the L1 norm. Several examples are presented: underdamped Langevin dynamics with variable diffusion matrices and three oscillator chain models with nearest-neighbor couplings, and underdamped mean field Langevin dynamics (weakly self-consistent Vlasov-Fokker-Planck equations).

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MS115

Online Learning in McKean-Vlasov SDEs and Interacting Particle Systems Using Single Trajectory Data

We introduce a new method for online parameter estimation in stochastic interacting particle systems, based on continuous observation of a single particle. Our method continuously updates the model parameters using a stochastic approximation of the gradient of the asymptotic log-likelihood. This gradient estimate, which is computed by simulating a set of synthetic interacting particles, is updated in parallel with the model parameters, converging asymptotically to the true direction of steepest ascent. Under suitable assumptions, we establish a.s. convergence of our method to the stationary points of the asymptotic log-likelihood, in the limit as the number of particles and the time horizon go to infinity. Under additional assumptions on the asymptotic log-likelihood function, we also establish an L2 convergence rate. Finally, we present several numerical examples, corroborating our theoretical results, and illustrating the robust performance of our estimator even in cases where our assumptions do not hold.

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MS115

On Resampling Schemes for Particle Filters with Weakly Informative Observations

We study the performance of different resampling schemes for particle filters in the context of hidden Markov models with "weakly informative" observations, which arise naturally in the context of time-discretizations of continuous-time Feynman-Kac models. Relatedly, we study the limiting behavior of these particle populations towards continuous-time interacting particle systems. Joint work with N. Chopin, S. S. Singh and M. Vihola.

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MS116

A Likelihood-Free Approach to Goal-Oriented Bayesian Experimental Design

Traditional Bayesian experimental design techniques often focus on maximizing the expected information gain (EIG) regarding model parameters. However, this approach may not always align with experimenters' objectives as it can be challenging to interpret and may not directly address their goals. In response, there is a growing need for goal-oriented experimental designs that directly cater to the experimenter's objectives. In this paper, we introduce a goal-oriented optimal experimental design (GO-OED) framework by considering EIG as a function of the experimenter's goal. Our approach seeks to identify a design that maximizes the reduction in entropy from the prior distribution of the goal function to its posterior distribution, considering all potential experimental outcomes. To tackle the computational complexity of efficiently computing EIG across various design points, we propose a novel method that avoids the need for likelihood evaluations or density computations. We employ Approximate Bayesian Computation (ABC) to obtain the posterior distribution, and we leverage density ratio estimation techniques to evaluate the utility of goal-oriented designs. We demonstrate the effectiveness of our approach through practical examples.

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MS116

Bayesian Model Averaging with Exact Inference of Likelihood- free Scoring Rule Posteriors

A novel application of Bayesian Model Averaging to generative models parameterized with neural networks (GNN) characterized by intractable likelihoods is presented. We leverage a likelihood-free generalized Bayesian inference approach with Scoring Rules. To tackle the challenge of model selection in neural networks, we adopt a continuous shrinkage prior, specifically the horseshoe prior. We introduce an innovative blocked sampling scheme, offering compatibility with both the Boomerang Sampler (a type of piecewise deterministic Markov process sampler) for exact but slower inference and with Stochastic Gradient Langevin Dynamics (SGLD) for faster yet biased posterior inference. This approach serves as a versatile tool bridging the gap between intractable likelihoods and robust Bayesian model selection within the generative modelling framework.

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MS116

ABC for Large Networks

Standard Approximate Bayesian Computation (ABC) methods provide alternative sampling algorithms for estimating the approximate posterior distribution of parameters of models defined by intractable likelihoods, while mainly requiring only the ability to efficiently draw dataset samples from the likelihood given proposed parameters, and to efficiently compute summary statistics on these sampled datasets. They include Exponential Random Graph Models and mechanistic models for networks. However, for the task of analyzing a very large network, it is computationally costly to simulate large networks from such a network model, and to compute and select relevant summary statistics on such networks. To address these issues, we propose a novel ABC algorithm that can provide sampling-based inferences from the posterior distribution of high-dimensional parameters of the given network model, while automatically selecting summary statistics relevant to the model. This ABC algorithm makes use of network-size-invariant summary statistics, which provide efficient sampling of, and summary statistics calculations on, network datasets smaller than the observed large network dataset being analyzed, while ensuring comparability between the simulated-dataset summaries and the observed-dataset summaries. These new ABC methods are illustrated through the analysis of large and multi-layered network data, while the methods can be extended to other intractable likelihood models.

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MS116

Reliable Likelihood-Free Inference Through Valid Confidence Regions

Many areas of science make extensive use of computer simulators that implicitly encode likelihood functions of complex systems. Classical statistical methods are poorly suited for these so-called likelihood-free inference (LFI) inverse problems, particularly with high-dimensional data and outside asymptotic regimes. In this talk I will present a new LFI framework that offers a practical and computationally efficient procedure for constraining parameters of interest that scales to complex high-dimensional data. The method also provides diagnostic tools to check whether the uncertainty estimates are indeed calibrated. In addition, our approach is compatible with general machine learning techniques that estimate likelihood or posteriors, and is amortized, meaning that no retraining is needed for new observed data. I will show advantages of this method and compare it with other popular tools in the modern ABC and posterior estimation literature.

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MS117

Fast Low-Rank Approximation of Parameter-Dependent Matrices

Many techniques for data science and uncertainty quantification demand efficient tools to handle Gaussian random fields. Quite often, these Gaussian random fields are defined in terms of parametrized covariance operators. In order to sample efficiently from such a random field for a range of parameters it is advantageous to perform low-rank approximation. In this talk, we discuss two different techniques for the more general problem of performing low-rank approximation for parameter-dependent matrices. The first approach is based on an extension of the so called adaptive cross approximation method, which is very well suited for isotropic covariance kernels, such as Matrn kernels. The numerical results demonstrate its advantages in terms of computational time and confirm that the proposed algorithm provides the basis of a fast sampling procedure. The second approach is based on an extension of randomized techniques, such as the randomized SVD and the Nystroem approximation, to a parameter-dependent setting.

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MS117

Error Estimation in Randomized Algorithms for Rank-Revealing Factorizations

Many problems in data science and scientific computing involve matrices that are dense but "data-sparse' and can be approximated by matrices of lower rank. In many applications, it is useful to work with a low-rank approximation that enables data interpretation in the same context as the original matrix. Interpolative decompositions (IDs) are well-suited for these types of problems because they involve

natural bases of row and column subsets of the matrix, known as skeletons, that approximately span its row and column spaces. For large problems, randomized sketching to sample the row or column space with a small random matrix can serve as an effective initial step in constructing IDs. A well-established method of skeleton selection for IDs is applying column-pivoted QR (CPQR) to random sketches, which has the added benefit of easily being made adaptive when the target rank for the approximation is unknown a priori. However, CPQR is more expensive and difficult to parallelize than algorithms based on LU with partial pivoting (LUPP), but a major drawback of LUPP is its well-known failure to be rank-revealing in the deterministic setting, making it challenging to build an adaptive algorithm for IDs based on LUPP. In this talk, we describe an adaptive, parallelizable algorithm based on LUPP applied to random sketches to determine a target rank for the ID approximation that leverages an efficient and reliable method of approximation error estimation. Our algorithm exhibits improved performance over algorithms that compute the ID with CPQR while maintaining comparable accuracy.

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MS117

Efficient Randomization Techniques for Data Assimilation

Strong Constraint 4D Variational (SC-4DVAR) is a data assimilation method that has applications in areas such as numerical weather prediction, etc. Computing the maximum a posteriori estimate in SC-4DVAR involves solving a minimization problem which we tackle using the Gauss-Newton Method. The computation of the descent direction is expensive since it involves a large linear solve of an ill-conditioned linear system. To address this cost, we efficiently construct scalable preconditioners using three different randomization techniques. The randomized techniques rely on a certain low-rank structure involving the Gauss-Newton Hessian. We also develop an adaptive approach to estimate the rank and to determine when to recompute the preconditioner. The proposed techniques are amenable to parallelization and drastically reduce the number of (Gauss-Newton) Hessian products. The proposed techniques also come with theoretical guarantees on the condition number. We demonstrate the performance and effectiveness of our methodology on the Burgers and quasi-geostrophic equations.

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MS118

Efficient Computation of Extreme Event Statistics with Generative Diffusion Models

Using generative models as emulators for the numerical simulations of dynamical systems is an appealing method for reducing the overall computational expense of sampling trajectories. This is particularly advantageous when dealing with tail events, which appear only rarely in direct numerical simulations, allowing the cost of training a generative model to be amortized over repeated use. We demonstrate how score-based diffusion models can serve as emulators for trajectories on the attractors of dynamical systems with a focus on accurate estimation of event probabilities. We further illustrate that a pre-trained diffusion model can be leveraged to sample exactly from a distribution which emphasizes tail events. This allows for the computationally efficient generation of such events. Finally, we present results using an emulator to generate and quantify the probability of extreme events unseen in the training data.

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MS118

Representation Learning with Denoising Diffusion Models for Geophysical Systems

The recent success of image genera1on, e.g., in DALL-E 3 or Stable diffusion, is linked to the emergence of deep generative modeling with (denoising) diffusion models. A neural network is trained to denoise diffused training samples. Iteratively applied, the neural network can map samples from a normal distribution to new data points. We demonstrate here results to the Lorenz 1963 system and a state-of-the-art high-resolution sea-ice model. These results indicate that diffusion models can be trained to generate states that are almost indistinguishable from simulations with such models. The diffusion model hereby learns an internal representation of the system. We exploit this internal representation and condition the diffusion model on simulated data by partial diffusion. During inference, a data sample is par1ally diffused and denoised. As the partial diffusion is inherently stochastic, we can generate many samples from a single data sample. This allows us to generate an ensemble out of a deterministic forecast. We test this approach for data assimilation in an ensemble optimal interpolation approach. Therein, so-generated ensemble members can outperform members drawn from a tuned, static background covariance matrix. We attribute this improvement to the ability of representing non-Gaussian distributions, an advantage compared to ensemble genera1on with covariance matrices. Therefore, we see a great potential of representation learning with diffusion models.

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MS118

Debias Coarsely, Sample Conditionally: Statistical Downscaling Through Optimal Transport and Probabilistic Diffusion Models

We introduce a two-stage probabilistic framework for statistical downscaling between unpaired data. Statistical downscaling seeks a probabilistic map to transform low-resolution data from a biased coarse-grained numerical scheme to high-resolution data that is consistent with a high-fidelity scheme. Our framework tackles the problem by composing two transformations: a debiasing step that is performed by an optimal transport map, and an

upsampling step that is achieved by a probabilistic diffusion model with a posteriori conditional sampling. This approach characterizes a conditional distribution without the need for paired data, and faithfully recovers relevant physical statistics from biased samples. We demonstrate the utility of the proposed approach on one- and two-dimensional fluid flow problems, which are representative of the core difficulties present in numerical simulations of weather and climate. Our method produces realistic high-resolution outputs from low-resolution inputs, by upsampling resolutions of 8 and 16. Moreover, our procedure correctly matches the statistics of physical quantities, even when the low-frequency content of the inputs and outputs do not match, a crucial but difficult-to-satisfy assumption needed by current state-of-the-art alternatives.

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MS119

Uncertainty Quantification Using Reduced-Basis Methods with Application to High Speed Flows

High-speed aerospace engineering applications rely heavily on computational fluid dynamics (CFD) models for design and analysis due to the expense and difficulty of flight tests and experiments. This reliance on CFD models necessitates performing accurate and reliable uncertainty quantification (UQ) to ensure that design and analysis decisions correctly incorporate the deficiencies of CFD models. However, it is very computationally expensive to run CFD for hypersonic flows due to high grid resolution requirements. Additionally, UQ approaches are many-query problems requiring many runs with a wide range of input parameters. This talk presents the use of the reduced-basis method for propagating parametric uncertainties with application to high-speed flows solved with the ReynoldsAveraged Navier-Stokes equations. We discuss a greedy algorithm that leverages novel, easily computable, error estimates for constructing a reduced basis. This reduced basis is used to define a Galerkin reduced-order model that leverages entropy-variable transforms to maintain robustness. We embed our reduced-order model within UQ approaches including multifidelity Monte Carlo and polynomial chaos workflows. We assess the utility of the reduced-basis method for more efficiently propagating parametric uncertainties in the SpalartAllmaras turbulence model. Results are presented on several high-speed turbulent flows. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

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MS119

Control-Theoretic Physics-Infused Reduced-Order Modeling with Infinite-Dimensional Parametric Inputs

The ever-lasting need for better systems in science and engineering pushes forward the quest for more scalable, efficient, and accurate models for design, analysis, optimization, and uncertainty quantification (UQ) of non-linear dynamical systems. Despite the existence of various successful reduced-order modeling techniques, e.g., projection-based methods and physics-informed machine learning, it remains a challenge to develop an efficient and accurate model that supports infinite-dimensional or distributed parameters. To resolve the challenge, we developed the Physics-Infused Reduced-Order Modeling (PIROM) that integrates the human knowledge and data through a physically consistent and UQ compatible manner. The PIROM builds upon a set of low-fidelity physics-based differential-algebraic equations compatible with distributed parameters, and augments the physics-based model with data-driven hidden dynamics to correct for its inherent inaccurate assumptions. The PIROM extends the incorporation of physical knowledge beyond inductive, learning, and observational biases to a new physics bias; this not only strongly restricts the model prediction onto the physics-consistent manifold for enhanced model generalizability, but also maintains the support for distributed parameters for complex optimization and UQ tasks. The talk will include the formulation, benchmark and demonstrations of the new PIROM methodology.

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MS119

Registration-Based Model Reduction of Shock-Dominated Flows

We propose an automated nonlinear model reduction and mesh adaptation framework for rapid and reliable solution of parameterized advection-dominated problems, with emphasis on compressible flows. The key ingredients of the method are threefold: (i) a metric-based mesh adaptation technique to generate an accurate mesh for a range of parameters, (ii) a general (i.e., independent of the underlying equations) registration procedure for the computation of a mapping Φ that tracks moving features of the solution field, and (iii) an hyper-reduced least-square Petrov-Galerkin reduced-order model for the rapid and reliable estimation of the mapped solution. The talk focuses on the problem of registration in complex geometries: we introduce a class of compositional maps that enable non-trivial deformations over curved boundaries of the domain; we develop a thorough analysis of the proposed ansatz for polytopal domains and we discuss the approximation properties for general curved domains. We present results for a parametric steady-state shock dominated flow to illustrate the performance of the method.

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MS120

Gaussian Process Regression: New Hyperparameter Estimation Algorithm for More Reliable Prediction

In the framework of the emulation of CPU-time expensive numerical simulators with Gaussian process (GP) regression, we propose in this work a new algorithm for the estimation of GP covariance parameters, referred to as GP hyperparameters. The objective is twofold: to ensure a GP as predictive as possible w.r.t. to the output of interest, but also with reliable prediction intervals, i.e. representative of GP prediction error. To achieve this, we propose a new constrained multi-objective algorithm for the hyperparameter estimation. It jointly maximizes the likelihood of the observations as well as the empirical coverage function of GP prediction intervals, under the constraint of not degrading the GP predictivity. Cross validation techniques and advantageous update GP formulas are notably used. The benefit brought by the algorithm compared to standard algorithms is illustrated on a large benchmark of analytical functions (with dimensions from 1 to 20 input variables). Different designs of experiments and different covariance models are considered. An application on a real data test case modeling an aquatic ecosystem is also proposed: GP metamodeling within a log-kriging approach is used to predict the biomass of a species at a given time. The multi-objective algorithm performs better than standard algorithms and this particular metamodeling framework shows the crucial interest of well-estimated and reliable prediction variances in GP regression.

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MS120

A Gradient-Enhanced Neural Network as a Surrogate for Elastoplastic Finite Element Analysis

When performing uncertainty quantification or optimization of an observed system, it is often necessary to evaluate the associated response repeatedly. This task can be solved by using complex numerical representations like finite element models, which can become time consuming and computationally expensive. Artificial neural networks show to be appropriate surrogate models for such repeated evaluations as well, thereby providing an alternative to the complex numerical models. In general, artificial neural networks are constructed using function values paired with input values during supervised training. When incorporating sensitivity information w.r.t. certain model parameters of these observed systems, additional gradient data is available. Thus, this contribution focuses on how to exploit the additional gradient information to train neural networks. The method of including gradient data into an artificial neural network follows by augmenting the inherent loss function used during training of the network model. Doing so, the supervised training process pairs function values and gradient values to input values. When taking advantage of this additional gradient data, the training and final performance of these gradient-enhanced artificial neural networks can be improved. The results show that gradient-enhanced artificial neural networks outperform the basic artificial neural networks during training, with better accuracy and quicker convergence of the training process.

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MS120

Physics-Informed Machine Learning for Surrogate Modeling of High-Dimensional Problems

We develop a physics-informed approach to efficiently construct and improve surrogate models for high dimensional input and output. In the proposed method, the dominant principal features of the output are identified using singular value decomposition. Active subspace discovery is used to map the input to a low-dimensional subspace, and surrogate models are built within the reduced spaces. Next, an active learning strategy in the low-dimensional latent space is developed to adaptively improve the surrogate model, with a novel learning function balancing exploration and exploitation. A third step is the incorporation of physical observations to further improve the surrogate model. An additive discrepancy term is introduced in the latent space to account for the inadequacy of each surrogate model. The posterior distributions of the discrepancy terms, model parameters and the observation errors are estimated based on measured output quantities, and then used for uncertainty quantification in the prediction of the unmeasured quantities. The proposed method is demonstrated on an additively manufactured component, with a high-dimensional field output quantities of interest, namely temperature and residual stress that have spatial variability due to the stochastic nature of process inputs and material properties.

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MS120

Adaptive Designs for Multi-Output Polynomial Chaos Expansions and Sensitivity Analysis

Adaptive design of experiments has been demonstrated very effective in reducing the computational costs of complex uncertainty quantification tasks, such as reliability and sensitivity analysis. While traditionally associated with local- and kernel- based surrogate models like Gaussian process modelling and support vector machines, recent research has demonstrated that adaptive design of experiments can also benefit regression- based surrogate models, such as polynomial chaos expansions (PCEs). Nevertheless, one core limitation of most adaptive design strategies is that, with few exceptions, they are designed for scalar-output models only. When dealing with multiple output models, optimality conditions become much more difficult to define, and the literature on the subject is still sparse. In this contribution, we extend a recently proposed semi-supervised sequential design approach for sparse PCE, to the case of vector-output computational models. Thanks to

the well-known synergy between PCE and Sobol' indices-based sensitivity analysis, this design of experiments strategy is also well suited for sensitivity analysis applications. We demonstrate the performance of this sequential design strategy on a number of well-known benchmarks from the surrogate modelling and sensitivity analysis literature.

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MS121

Mean-Field Ensemble Kalman Methods: Gaussian and Particle Approximations

The ensemble Kalman methodology is an innovative and flexible set of tools which can be used for both state estimation in dynamical systems and parameter estimation for generic inverse problems. It has primarily been developed by practitioners in the geophysical sciences, yet, despite its widespread adoption in fields of application, firm theoretical foundations are only now starting to emerge. We consider a unifying approach to algorithms that rests on transport of measures and mean-field stochastic dynamical systems. The ensemble Kalman methods as implemented in practice rely on projections onto the space of Gaussian measures and particle approximations. With the goal of developing theoretical guarantees for the ensemble Kalman methodology applied to non-linear problems, we discuss the error analysis and ergodicity of the mean-field stochastic dynamical systems arising in ensemble Kalman filtering, along with Gaussian and particle approximations.

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MS121

Non-linear Analysis of the Localized Ensemble Kalman-Bucy Filter with Sparse Observations

With large scale availability of precise real time data, their incorporation into physically based predictive models, became increasingly important. This procedure of combining the prediction and observation is called data assimilation. One especially popular algorithm of the class of Bayesian sequential data assimilation methods is the ensemble Kalman filter which successfully extends the ideas of the Kalman filter to the non-linear situation. However, in case of spatio-temporal models one regularly relies on some version of localization, to avoid spurious oscillations. In this work we develop a-priori error estimates for a time continuous variant of the ensemble Kalman filter, known as localized ensemble Kalman–Bucy filter. More specifically we aim for the scenario of sparse observations applied to models from fluid dynamics and space weather.

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MS121

The Mean Field Ensemble Kalman Filter: Near-Gaussian Setting

The ensemble Kalman filter is widely used in applications because, for high dimensional filtering problems, it has a robustness that is not shared for example by the particle filter; in particular it does not suffer from weight collapse. However, there is no theory which quantifies its accuracy as an approximation of the true filtering distribution, except in the Gaussian setting. To address this issue we provide an analysis of the accuracy of the ensemble Kalman filter beyond the Gaussian setting. Our analysis is developed for the mean field ensemble Kalman filter. We rewrite the update equations for this filter, and for the true filtering distribution, in terms of maps on probability measures. We introduce a weighted total variation metric to estimate the distance between the two filters and we prove various stability estimates for the maps defining the evolution of the two filters, in this metric. Using these stability estimates we demonstrate that if the true filtering distribution is close to Gaussian in the joint space of state and data, in the weighted total variation metric, then the true-filter is well approximated by the ensemble Kalman filter, in the same metric.

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MS121

Gradient Flow Structure and Convergence Analysis of the Ensemble Kalman Inversion

The ensemble Kalman filter (EnKF) is a widely used methodology for data assimilation problems and has been recently generalized to inverse problems, known as ensemble Kalman inversion (EKI). We view the method as a derivative-free optimization method for a nonlinear least-squares misfit functional and discuss various variants of the scheme such as covariance inflation and regularization. This opens up the perspective to use the method for a wide range of applications, e.g. imaging, groundwater flow prob-

lems, biological problems as well as in the context of the training of neural networks. Based on the continuous time formulation we quantify the gradient flow structure of the scheme and present accuracy results of the EKI estimate.

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MS122

Shape Uncertainty for Cardiac Reconstruction with Signed Distance Functions

The efficient construction of an anatomical model is one of the major challenges of patient-specific in-silico models of the human heart. Current methods frequently rely on linear statistical models, allowing no advanced topological changes, or requiring medical image segmentation followed by a meshing pipeline, which strongly depends on image resolution, quality, and modality. These approaches are therefore limited in their transferability to other imaging domains. In this work, the cardiac shape is reconstructed by means of three-dimensional deep signed distance functions with Lipschitz regularity. For this purpose, the shapes of cardiac MRI reconstructions are learned from public databases to model the spatial relation of multiple chambers in Cartesian space. We demonstrate that this approach is also capable of reconstructing anatomical models from partial data, such as point clouds from a single ventricle, or modalities different from the trained MRI, such as electroanatomical mapping, and in addition, allows us to generate new anatomical shapes by randomly sampling latent vectors. Finally, we quantify the shape uncertainty using multilevel Markov chain Monte Carlo methods.

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MS122

Quantifying Domain Uncertainty in Linear Elasticity

The numerical solution of the equations of linear elasticity is well understood if the input parameters are known. This, however, is often not the case in practical applications. In this talk uncertainties in the description of the computational domain is considered. To this end, we model the random domain as the image of some given fixed, nominal domain under random domain mapping. We then prove the analytic regularity of the random solution with respect to the countable random input parameters which enter the problem through the Karhunen-Love expansion of the random domain mappings. In particular, we provide appropriate bounds on arbitrary derivatives of the random solution with respect to those input parameters, which enable the use of state-of-the-art quadrature methods to compute quantities of interest such as the mean and variance of the random von Mises stress in a dimensionally robust way.

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MS122

***p*-multilevel Monte Carlo for Acoustic Scattering from Large Deviation Rough Random Surfaces**

We study time harmonic acoustic scattering on large deviation rough random scatterers. Therein, the roughness of the scatterers is caused by a low Sobolev regularity in the covariance function of their deformation field. The motivation for this study arises from physical phenomena where small-scale material defects can potentially introduce nonsmooth deviations from a reference domain. The primary challenge in this scenario is that the scattered wave is also random, which makes computational predictions unreliable. Therefore, it is essential to quantify these uncertainties to ensure robust and well-informed design processes. While existing methods for uncertainty quantification typically rely on domain mapping or perturbation approaches, it turns out that large and rough random deviations are not satisfactory covered. To close this gap, and although counter intuitive at first, we show that the p-multilevel Monte Carlo method can provide an efficient tool for uncertainty quantification in this setting. To this end, we discuss the stable implementation of higher-order polynomial approximation of the deformation field by means of barycentric interpolation and provide a cost-to-accuracy analysis. Our considerations are complemented by numerical experiments in three dimensions on a complex scattering geometry.

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MS122

A pCN-MCMC Method for a Bayesian Inverse Problem in Nanoscale Devices

Nanoscale semiconductor devices have many applications ranging from cybersecurity to medicine and healthcare. In this talk, we formulate a Bayesian inverse problem for a PDE model of semiconductors, in which the goal is to reconstruct the uncertain doping profile. To solve this infinite-dimensional Bayesian inverse problem, we deploy a Markov-chain Monte-Carlo method with a preconditioned Crank-Nicolson proposal, where we use a physics-informed prior knowledge to estimate the posterior distribution of the doping function. We present the numerical results of the reconstruction from the voltage-current measurements

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MS123

An Overview of Monte Carlo and Machine Learning Methods for Solving PDEs

This talk will give an overview of Monte Carlo and machine learning techniques for solving partial differential equations. There are non-deterministic techniques, and we will give a brief overview and the discuss the pros and cons of these methods.

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MS123

Walking Forward and Backward in Euler Schemes and Random Number Generators

I will present how to take advantage of the reversibility of some Random Number Generators to resampling the path of Euler approximations of a SDE. Doing so, this induces an additional error $(1/N)$ which we prove to be smaller than the one for forward sampling $(1/\sqrt{N})$, with respect to the number of time steps N . The method allows in particular to retrieve sampled points with a minimal amount of information. It can be used in regression Monte Carlo methods for memory saving concerns.

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MS124

Calibration of High-Dimensional Models Through Linked Emulators

We present the calibration of a pulmonary simulator through history matching. Due to the cost of the model, an emulator is required. The model is high dimensional because it depends on simulating the alveoli in the lungs individually. Each alveolar unit depends on three inputs and each one of these units contributes equally to the model output, for which naive dimension reduction is ineffective. We solve this problem by dividing the process into two emulators, the second one taking the output of the first one as its inputs, thereby linking them. We show that this strategy is a feasible solution for models with a high-dimensional input, where each input contribution is such that no identification of active variables is possible. We also explore connections with deep Gaussian processes.

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MS124

Model Discrepancy for Uncertainty Quantification

When assessing uncertainty for complex physical systems which are represented by computer simulators, a crucial feature relates to the structural discrepancy, i.e. the mismatch between the model and the system even at appropriate choices of the model parameters. In this talk, we will focus on systematic methods for quantifying model discrepancy, distinguishing between internal discrepancy (those features that we can learn about by experiments on the model itself) and external discrepancy (those features arising from aspects of the real world system that are not represented within the model). The talk will be general but examples and illustrations will relate to the themes of the workshop.

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MS124

Global Sensitivity Analysis of Stochastic Models: Challenges

The sensitivity analysis of stochastic models poses mathematical, and even philosophical, challenges. On the one hand, we may think of a stochastic model as a collection of probability laws. However, this viewpoint raises several issues. First, these probability laws are not observable; only samples can be drawn. This raises inference questions, because one often needs repetitions of the model and hence increases the computation cost dramatically. Second, distinct functionals of these laws correspond to distinct sensitivity indices, and it is unclear which should be used. Finally, the sensitivity to the endogenous variability of the stochastic model cannot be assessed. On the other hand, it can be argued that every stochastic model is, after all, nothing more than a computer program, and hence completely deterministic. But then, as we shall see, the values of the sensitivity indices depend on the algorithm used to simulate the model. The above challenges will be discussed in more details and illustrated on SIR-like models. Possible avenues for future research will be proposed.

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MS124

Markov Chain Monte Carlo Methods for Electrical Conductivity Estimation in the Heart

Cardiac arrhythmias are caused by abnormal or irregular electrical activity in the heart and are a leading cause of stroke. The exact pathophysiology of a cardiac arrhythmia differs significantly between individuals requiring patient-specific treatment. Precision cardiology aims to achieve this by creating patient-specific models of cardiac electrophysiology. State-of-the-art imaging techniques still limit the precision with which we can describe the heart of an individual. As a consequence, uncertainty quantification on the predictions made by the resulting model is of interest. Motivated by the case of ventricular tachycardia caused by reentry because of inhomogeneities in the tissue conductivity, we propose a Markov chain Monte Carlo method in this talk to obtain a Bayesian posterior distribution of the space-dependent (and thus high-dimensional) electrical conductivity in a Mitchell-Schaeffer description of a 2D tissue slab. To evaluate the methods performance, we mimic sparse electrocardiogram data synthetically. A major issue is that, on top of the sparsity of the available data and its associated measurement error, the data is sub-

ject to significant intra-individual variability, which needs to be accounted for when defining an appropriate likelihood function. We will show the effect of different choices for the likelihood function and the noise model on the obtained posteriors and provide insight in the effect of model error on the uncertainty of the predictions.

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MS125

Probabilistic Numerics for Ordinary Differential Equations

Probabilistic numerical methods aim to explicitly represent the numerical uncertainty that results from finite computational resources. In this talk, we present a flexible and efficient class of probabilistic numerical solvers for ordinary differential equations (ODEs) based on Bayesian filtering and smoothing. By posing the numerical solution of an ODE as a Gauss–Markov regression problem, these so-called "ODE filters" efficiently compute posterior distributions over ODE solutions and thereby quantify the numerical approximation error. Additionally, their probabilistic formulation allows them to be taylored to the specific problem at hand, for example by choosing appropriate prior distributions or by incorporating additional information about the solution. The ideas presented in this talk open up new possibilities for accurate and efficient probabilistic simulation and inference in dynamical systems.

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MS125

PDE-Constrained Gaussian Processes and Kernels

Gaussian process regression (GPR) is the Bayesian formulation of kernel regression methods used in machine learning. This method may be used to treat regression problems stemming from physical models, the latter typically taking the form of partial differential equations (PDEs). In this presentation, we study the question of the design of GPR methods, in relation with a target PDE model. We first provide several necessary and sufficient conditions describing how to rigorously impose certain physical constraints (explicitly, the distributional PDE constraint if the PDE is linear, and the control of the $W^{m,p}$ Sobolev energy norm) on the realizations of a given centered Gaussian process. These results only involve the kernel of the Gaussian process. We then provide a simple application test case, with the estimation of the solution of the 3D wave equation (central in acoustics), as well as the estimation of the physical parameters attached to this PDE. If time allows, we will also describe explicit links between such physics-informed GPR models and classical numerical methods for solving PDEs, such as the finite difference method.

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MS125

Kernel methods for learning PDEs

We introduce a framework for learning partial differential equations (PDEs) using kernel methods. Our proposed method is accompanied with extensive theoretical results such as error bounds and convergence analysis as well as extensive numerical benchmarking. Given a training set consisting of pairs of noisy and limited observations of PDE solutions and source terms, we employ a graph completion approach towards learning the functional form of the underlying PDE via an optimal recovery approach in an RKHS. Our numerical experiments demonstrate that our approach is particularly competitive in the low-data regime where very few observations of the PDE solution and source terms are available.

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MS126

VC Dimension of GNNs with Pfaffian Activation Functions

Graph Neural Networks (GNNs) have emerged in recent years as a powerful tool to learn tasks across a wide range of graph domains in a data-driven fashion; based on a message passing mechanism, GNNs have gained increasing popularity due to their intuitive formulation, closely linked with the Weisfeiler-Lehman (WL) test for graph isomorphism, to which they have proven equivalent. From a theoretical point of view, GNNs have been shown to be universal approximators, and their generalization capability (namely, bounds on the VC dimension) has recently been investigated for GNNs with piecewise polynomial activation functions. The aim of our work is to extend this analysis on the VC dimension of GNNs to other commonly used activation functions, such as sigmoid and hyperbolic tangent, using the framework of Pfaffian function theory. Bounds are provided with respect to the usual parameters (depth, number of neurons, input size) as well as with respect to the number of colors resulting from the 1-WL test applied

on the graph domain. The theoretical analysis is supported by a preliminary experimental study.

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MS126

Bifurcation Diagrams of PDEs with Parametric Uncertainty

Complex physical phenomena can often be described by PDEs with random coefficients, possibly involving a large number of uncertain parameters. Crucially, the presence of such uncertainty might render into very different behavior of the modeled phenomenon, e.g. due to the randomness of the stability region of an equilibrium. In this talk, we consider model equations such as the Allen-Cahn equation with polynomial nonlinearity. We take a look at bifurcation diagrams and regard them as random objects, meaning that e.g. equilibria and bifurcation points are random quantities. As such, they call for uncertainty quantification methods. In particular, we investigate the forward uncertainty quantification problem, i.e. the propagation of the uncertainty of the model coefficients to such quantities by means of sparse grids and the polynomial chaos method.

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MS126

Neural Operators for Gaussian Random Field Inputs

In this talk we discuss the use of operator surrogates to approximate smooth maps between infinite-dimensional Hilbert spaces. Such surrogates have a wide range of applications in uncertainty quantification and parameter estimation problems. The error is measured in the L^2-sense with respect to a Gaussian measure on the input space. Under suitable assumptions, we show that algebraic and dimension-independent convergence rates can be achieved.

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MS126

Locality in Sparse Polynomial Approximation of Parametric PDEs and Application to Parameterized Domains

We study how the choice of the representation of a parametric, spatially distributed boundary of an elliptic partial differential equation affects the efficiency of a polynomial surrogate for the parameter-to-solution map for the solution on a reference configuration. We focus on the possible improvements in convergence rates by exploiting locality in the basis expansion of the domain. We show theoretically that, for basis expansions that exhibit certain locality properties and some mappings to the reference configuration, the convergence rate of polynomial surrogates improves when compared to globally supported basis functions. Moreover, we perform extensive numerical experiments to show this result for mollifier and PDE-based mappings, uncovering differences in the convergence behavior between both mappings.

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MS127

Physics-consistency of Infinite Neural Networks

Recent research has highlighted the incorporation of prior physics knowledge into neural networks (NNs) beyond the well-known approach of regularizing physics-information in the optimization objective. Here in particular, we aim at the construction of special neural activation functions. For this, we consider (i) Gaussian process (GP) kernels that adhere to the principles of physics, and (ii) the infinite-width correspondence between NNs and GPs. Together, this begs the question for infinite-width NNs that are consistent with the laws of physics. So construed regression models may find specialized applications such as inverse problems, uncertainty quantification. These surrogate models should learn efficiently from limited data while generalizing in a physically sensible manner. We start with a simple single-layer NN, albeit the infinite-width correspondence holds for general deep feedforward or recurrent architectures. Under certain conditions and in the infinite-width limit, we may apply the central limit theorem. We may then investigate and manipulate the limit network by falling back on GP theory. It is observed that linear operators acting upon a GP again yield a GP. This also holds true for differential operators defining differential equations and describing physical laws. If we demand the GP, or equivalently the limit network, to obey the physical law, then this yields an equation for the physics consistency of the covariance function.

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MS127

Information Field Theory Based Reconstruction of Radio Signals from Atmospheric Particle Cascades

Cosmic rays are highly energetic particles traversing the

universe at relativistic speeds. When they hit the Earth's atmosphere, they create a particle cascade. In this cascade, charges are separated, emitting radio waves, which can be measured with antenna arrays. Unfortunately, the noise underlying the measurements can impact the quality of the reconstruction of the cascade. Information Field Theory (IFT) can be used to infer the true signal from the noisy measurements. It is based on Bayesian statistics and introduces numerical methods to efficiently apply it to high dimensional fields even without precise knowledge of the prior distribution. By simply knowing the correlation structure of the field, which is to be reconstructed, Information Field Theory provides methods to approximate the posterior distribution, even for non-linear systems. More specifically, Metric Gaussian Variational Inference (MGVI) approximates the true posterior distribution with a Gaussian. As MGVI does not only find the maximum likelihood solution, but rather approximates the posterior, it is also possible to obtain uncertainty estimates from it.

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MS127

UBIK - The Universal Bayesian Imaging Kit

The advent of the next generation of measurement instruments in astrophysics and elsewhere poses several challenges due to the high-dimensional signals that vary in space, time, and energy. These have typically non-trivial correlation structures and are often a mixture of overlapping signals that must be separated. In order to facilitate the multi-instrument analysis of superimposed, correlated signals in general, we develop the Universal Bayesian Imaging Kit (UBIK), a flexible and modular framework for high-fidelity Bayesian imaging. UBIK is designed to address these challenges using Information Field Theory, a theoretical framework for the consistent application of Bayesian logic to signal reconstruction. UBIK uses generative models to encode prior knowledge about the signals of interest in order to exploit spatial, temporal, and spectral correlations to improve their reconstruction from noisy data. Moreover, the fully Bayesian inference description allows to estimate uncertainties. It comes with a growing set of instrument-specific likelihoods, which allows to combine datasets from different observations. Here, the current development status of UBIK is reported and its abilities are illustrated at the example of high-fidelity spatio-spectral visualization of complex emission structures in astrophysical objects reconstructed based on Poisson-noise-affected X-ray data from the Chandra and eROSITA satellites.

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MS128

Global Sensitivity Analysis for Rare Event Probabilities

Rare event probabilities are expensive to compute. They are also delicate to estimate because their value strongly depends on distributional assumptions on the model parameters. Therefore, understanding the sensitivity of the computed rare event probabilities to the hyper-parameters that define the distribution law of the model parameters is crucial. We show that by (i) accelerating the calculation of rare event probabilities through subset simulation and (ii) approximating the resulting probabilities through polynomial chaos expansions, the global sensitivity of such problems can be analyzed through a double-loop sampling approach. The resulting method is conceptually simple and computationally efficient. We test the performance of the proposed approach on a simple analytic example as well as a subsurface flow application.

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MS128

MLMC Techniques for Computing Probabilities

In this talk, I will discuss several Monte Carlo-based estimators for computing probablities and other discontious functional of random variables with approximate samples. The models we consider are arbitraly nested expectations as well as stochastic and partial differential equations. I will present our recent works on adaptive and path branching estimators based on Multilevel Monte Carlo (MLMC) which have a computational compelxity similiar to a classical Monte Carlo estimator with exact samples of the random variables. The talk is based on two papers:

- Haji-Ali, Spence, and Teckentrup. "Adaptive Multilevel Monte Carlo for Probabilities." SIAM Journal on Numerical Analysis 60.4 (2022): 2125-2149.
- Giles, Haji-Ali. "Multilevel path branching for digital options." arXiv preprint arXiv:2209.03017 (2022).

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MS128

Importance Sampling for McKean-Vlasov SDEs

We are interested in Monte Carlo (MC) methods for estimating probabilities of rare events associated with solutions to the McKean-Vlasov stochastic differential equation (MV-SDE). MV-SDEs arise in the mean-field limit of stochastic interacting particle systems, which have many applications in pedestrian dynamics, collective animal behaviour and financial mathematics. Importance sampling (IS) is used to reduce high relative variance in MC estimators of rare event probabilities. Optimal change of measure

is methodically derived from variance minimisation, yielding a high-dimensional partial differential control equation which is cumbersome to solve. This problem is circumvented by using a decoupling approach, resulting in a lower dimensional control PDE. The decoupling approach necessitates the use of a double Loop Monte Carlo (DLMC) estimator. We further combine IS with a novel multilevel DLMC estimator which not only reduces complexity from O(TOL-4) to O(TOL-3) but also drastically reduces associated constant, enabling computationally feasible estimation of rare event probabilities.

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MS128

Large Deviation Theory-Based Adaptive Importance Sampling for Rare Events in High Dimensions

Rare and extreme are infrequent but have severe consequences. Estimating the probability of such events can inform strategies that mitigate their effects. However, calculating small probabilities is hard, particularly when involving complex dynamics and high-dimensional random variables. In this talk, I will discuss our proposed method for accurately estimating rare event or failure probabilities for expensive-to-evaluate numerical models in high dimensions. The proposed approach combines ideas from large deviation theory and adaptive importance sampling. The importance sampler uses a cross-entropy method to find an optimal Gaussian biasing distribution, and reuses all samples made throughout the process for both, the target probability estimation and for updating the biasing distributions. Large deviation theory is used to find a good initial biasing distribution through the solution of an optimization problem. Additionally, it is used to identify a low-dimensional subspace that is most informative of the rare event probability. This subspace is used for the cross-entropy method, which is known to lose efficiency in higher dimensions. We compare the method with a state-of-the-art cross-entropy-based importance sampling scheme using examples including a high-dimensional failure probability estimation benchmark and a tsunami problem governed by the time-dependent shallow water system.

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MS129

A Reinforcement Learning and Variational Approach to Sequential Optimal Experimental Design

We introduce variational sequential Optimal Experimental Design (vsOED), a new method for optimally designing a finite sequence of experiments under a Bayesian framework and with information-gain utilities. Specifically, we adopt a lower bound estimator for the expected utility through variational approximation to the Bayesian posteriors. The optimal design policy is solved numerically by simultaneously maximizing the variational lower bound and performing policy gradient updates. We demonstrate this general methodology for a range of OED problems targeting parameter inference, model discrimination, and goal-oriented prediction. These cases encompass explicit and implicit likelihoods, nuisance parameters, and physics-based partial differential equation models. Our vsOED results indicate substantially improved sample efficiency and reduced number of forward model simulations compared to previous sequential design algorithms.

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MS129

Bayesian Optimal Experimental Design: a Combinatorial Approach via Logarithmic Sobolev Inequalities

In this talk, we study the problem of selecting the most informative subset of k designs from a pool of N available options. The assessment of performance in this context is characterized by the mutual information between the observations and the underlying parameters. Obtaining the exact solution is of exponential complexity, requiring one to explore $\binom{N}{k}$ possible combinations. To overcome this challenge, we introduce a method to attain an approximate solution by optimizing over an upper bound on the difference between the mutual information, where the proposed upper bound is constructed via the log-Sobolev inequality. We demonstrate that our method outperforms the random selection strategies and the Gaussian approximations in the nonlinear settings using numerical examples.

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MS129

Consistency of Some Sequential Experimental Design Strategies for Excursion Set Estimation Based on Vector-Valued Gaussian Processes

We tackle the extension to the vector-valued case of consistency results for Stepwise Uncertainty Reduction sequential experimental design strategies established in [Bect et al., A supermartin- gale approach to Gaussian process based sequential design of experiments, Bernoulli 25, 2019]. This lead us in the first place to clarify, assuming a compact index set, how the connection between continuous Gaussian processes and Gaussian measures on the Banach space of continuous functions carries over to vector-valued settings. From there, a number of concepts and properties

from the aforementioned paper can be readily extended. However, vector-valued settings do complicate things for some results, mainly due to the lack of continuity for the pseudo-inverse mapping that affects the conditional mean and covariance function given finitely many pointwise observations. We apply obtained results to the Integrated Bernoulli Variance and the Expected Measure Variance uncertainty functionals employed in [Fossum et al., Learning excursion sets of vector-valued Gaussian ran- dom fields for autonomous ocean sampling, The Annals of Applied Statistics 15, 2021] for the estimation for excursion sets of vector-valued functions.

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MS130

On the Statistical Properties of Embedded Inadequacy Models

Conventional Bayesian regression has no mechanism for addressing model form error. As the number of observations increases, the posterior distribution contracts around the most probable parameter values, conditioned on the assumed model. In practice, models are inadequate, and the spread of the posterior does not reflect this model inadequacy or misspecification. Attempts to characterize model form error with additive nonparametric discrepancy models can break physical laws or incur large computational expense. We instead present and analyze parametric embedded error models, which represent some subset of parameters in the original (inadequate) model as random variables with explicitly modeled stochastic dimensions. This approach implicitly modifies the likelihood function so that data which could not be explained as independent observations of the original model can instead be explained through correlated non-stationary observational errors. The embedded error model can also be interpreted as a modified representation of epistemic uncertainty through a strategic injection of aleatoric uncertainty. From a computational perspective, we will demonstrate that triangular transport maps can be used to calibrate such embedded error models, in the paradigm of simulation-based inference. From the statistical perspective, we will analyze the calibration and tails of the resulting predictive distributions.

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MS130

Efficient Model Uncertainty via the Laplace Approximation in Practice

Neural networks, renowned for their remarkable predictive accuracy, occasionally exhibit perplexing failures when confronted with data points seemingly akin to their training data. To instill confidence in the reliability of model predictions, it is imperative to quantify uncertainty effectively. Various methods, encompassing Markov Chain Monte Carlo (MCMC), variational inference, and ensemble techniques, offer uncertainty estimates for neural network outputs. Nonetheless, practical applications often demand simple and fast approximations, particularly suited for large or complex models. This functionality is provided by the Laplace approximation for neural networks, a method that uses a Gaussian approximation of the posterior distribution around the maximum a-posteriori estimate. In this study, we delve into the applications of the Laplace approximation, spanning across classification, neural Ordinary Differential Equations (ODEs), and numerical integration tasks. Our investigation focuses on models enriched with supplementary knowledge of the underlying data generation process, probing whether this additional information decreases uncertainty in model predictions.

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MS131

Enabling Bayesian Optimal Experimental Design for High-Dimensional Systems with Incremental Tensor Decompositions

Bayesian inference and other UQ analysis are extremely challenging in high-dimensional spaces. One common approach to mitigate these challenges is to perform dimension reduction in a way that enables inverse problems to be solved in the reduced latent space. In this presentation, we highlight a novel approach that incorporates Bayesian optimal experimental design with incremental tensor decompositions that address scalability challenges through multi-linear low-rank reduction. Using large-scale tensor-structured data (e.g. solutions of PDEs), we uncover a latent structure through incremental tensor decompositions. We then exploit the low rank tensor formats in determining the optimal sensor placement strategy. We demonstrate results through simulations on a chaotic PDE-driven system of self-oscillating gels and compare the quality-of-inference against different strategies in terms of inversion accuracy.

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MS131

Gauss-Newton-Inspired Approaches to Train Deep Neural Networks Efficiently

Deep neural networks (DNNs) have achieved inarguable success as high-dimensional function approximators in countless applications, including numerous scientific applications such as surrogate modeling, operator learning, and model discovery. However, this success comes at a significant hidden cost, notably a long training time. Typically,

training is posed as a stochastic optimization problem to learn the DNN weights. However, we can interpret training as solving a high-dimensional, nonlinear data fitting problem for which Gauss-Newton has traditionally been the go-to optimization strategy. Despite this tradition, Gauss-Newton has not gained widespread use for DNN training, often due to computational bottlenecks. In this talk, we propose a memory and computationally efficient Gauss-Newton implementation that can solve the training problem well and learn weights that generalize. We will describe how we obtain this efficiency by approximating the Jacobian with only a few additional passes through the network. We will demonstrate the computational advantages of our approach over traditional stochastic optimizers on several benchmark deep learning tasks.

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MS131

Adaptive Planning for Risk-aware Predictive Digital Twins

Rigorous mathematical foundations are crucial to develop robust and reliable digital twins in computational science and engineering. We propose a method to increase the personalization and robustness of digital twins through the use of a probabilistic graphical model formulation and parametric Markov decision processes with transition probabilities modelled as random variables. We incorporate probabilistic model-checking and linear programming into a dynamic Bayesian network to enable risk-averse adaptive mission replanning of an unmanned aerial vehicle. The proposed method allows to refine the optimal policy at every time step resulting in a better trade off between operational costs and performances. Employing random variables with a known distribution to model the transition probabilities enables us to easily compute risk measures to account for rare events connected to failures.

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MS132

Recent Progress in Model Ensemble Configuration for Multifidelity UQ

Multifidelity uncertainty quantification (MF UQ) can be an effective tool for quantifying the effects of statistical variability for expensive high-fidelity computational models. By integrating information from multiple models of varying accuracy and cost, accurate estimates of statistical quantities of interest can be obtained at significantly reduced expense relative to single-fidelity approaches. In practical deployments of these MF UQ methods, performance can be impeded by the need to select the best statistical estimators and to identify and optimally configure the most effective ensemble of lower fidelity approximations. In this work, we present recent findings in the optimal configuration of a model ensemble for multifidelity sampling, defined in terms of ensemble membership (the set of included approximations), model pairings or groupings (from DAG pairings or set enumerations), and approximation hyper-parameter settings (as determined by model tuning processes). Of particular interest is exploring solution approaches based on generalized ACV [Bomarito et al., J. Comput. Phys. 2022] and multilevel BLUE [Schaden and Ullmann, SIAM J. UQ 2020], expanded to include hyper-parameter model tuning. In aggregate, these developments target a more unified approach for ensemble management in MF UQ.

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MS132

Multi-Fidelity Sampling Estimators for Models with Dissimilar Parametrization

Multifidelity sampling estimators are effective in reducing the overall computational burden of uncertainty quantification (UQ) tasks. A variety of strategies, spanning multilevel and multi-fidelity approaches, have been proposed in the last couple of decades. The foundational idea of all these methods is to fuse a large number of low-fidelity evaluations with limited amounts of high-fidelity runs to obtain a larger precision of the estimator, while preserving the high-fidelity accuracy. Unfortunately, many of the existing methods still suffer from the degradation in correlation associated to the use of dissimilar parametrization among models. Dissimilar parametrizations arise quite naturally when dealing with complex computational problems in which either the parameters, or their distributions, are model-specif, e.g., they are associated to a particular physical model/closure not shared within the models ensemble. In this talk, we will present how dimension

reduction strategies can be used to identify and leverage the latent variables shared among models in order to enhance their correlation in these situations. We will present an array of test problems to illustrate the benefits of the proposed approach when compared with standard single-fidelity strategies. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

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MS132

Multifidelity Explorations of Non Equilibrium Flows Using Eigen Decomposition

When an aircraft operates at hypersonic speeds, compressibility effects lead to the formation of a strong bow shock, initiating a cascade of reactions that cause the gas to become chemically reactive. For the design of an effective Thermal Protection System (TPS), its essential to predict the gas state within this shock layer accurately. However, challenges arise due to uncertainties in chemical model parameters, model form discrepancies, and computational demands. State-to-state (StS) models offer high accuracy but are computationally intensive. Reduced-order models based on coarse-graining group chemical species simplify the process, but accuracy depends on cluster selection and reconstruction complexity. This work proposes a multi-fidelity surrogate model that combines abundant, less accurate low-fidelity simulations with a few accurate, expensive high-fidelity ones to create a dataset. This combined dataset is used to identify a low-dimensional subspace using eigen-decompositions. The eigen coefficients obtained therein train a Polynomial Chaos Expansion (PCE) with stochastic coefficients to account for model form uncertainty. This multi-fidelity surrogate model that combines the capabilities of eigendecomposition and PCE allows faster predictions of the full flow field at new locations in the uncertain input parameter and boundary condition space with excellent accuracy but at a much lower computational cost than the high-fidelity simulations.

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MS132

Multidifidelity Uncertainty Analysis of Laser-Induced Rocket Ignition: Experiments and Simulations

Computer simulations have widespread use as predictive tools in every field of science and engineering. Computations, traditionally, have been assumed to be accurate and ergo useful when consistent numerical schemes and algorithms are adopted, along with sufficient spatio-temporal fidelity in the case of scale-resolving simulations. However, for simulations to be predictive of real-world scenarios, uncertainties representing limited knowledge and precisions need to be accounted for, even in nominally controlled systems. Consequentially, algorithms that utilize an ensemble of simulations need to be considered to provide confidence in the predictions despite the uncertainties. This leads to an increase of the simulation throughput by orders of magnitude. In this talk, we discuss the use of simulation ensembles of quantities arising from laser-induced ignition in rocket engines. The outputs of interest in these problems often have abrupt, drastic and sudden changes in the measurements. We investigate a bi-fidelity approach with interpolative decomposition and study the reliability of this method. We also compare the prediction accuracy with non-linear bi-fidelity strategies based on autoencoders.

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MS133

Control of Kinetic Collective Dynamics by Deep Neural Feedback Laws

The modelling of multi agent systems (MAS) can be seen as the result of a suitable combination of with-in population interactions and external influences. We address how to successfully condition high dimensional MAS towards a designed cooperative goal (e.g. consensus) by means of dynamic optimization. The problem reads as the minimization of a cost functional subject to individual-based dynamics; thus, its solution easily becomes unfeasible as the number of agents grows. A natural way of circumventing this difficulty is by passing from a microscopic viewpoint to a macroscopic one, that is from an agent-to-agent description of the trajectories to the evolution of the system represented as a density in space and time. Although mean field optimal control problems are designed to be independent of the number of agents, they are feasible to solve only for moderate intrinsic dimensions of the agents' space. For this reason, we propose a procedure for approaching the solution from suboptimality by means of a Boltzmann scheme. We consider the quasi-invariant limit of binary interactions as approximation of the mean field PDE governing the dynamics of the agents distribution. This considerably tackles down the numerical complexity of the original problem, which is now reduced to a collection of many 2-agents sub-systems. The need for an efficient solver of the binary OCP motivates the use of Neural

Networks.

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MS133

Deterministic Estimation for Sub-differential Dynamics and Links with Stochastic Filtering

Stochastic filtering computes statistical properties of a random dynamics when conditioning by a noisy observation process, whereas deterministic observation produces an estimator by fitting a deterministic dynamics with observation. In their 1987 article, Baras and James proved that both procedures yield the same result as the noise amplitude is sent to zero. In this talk, we present the corresponding convergence result for sub-differential dynamics defined through variational inequalities. Using tools from control theory, the limit of the stochastic filter can be identified when the noise amplitude goes to zero. Following Mortensens method, we then define a causal estimator for the deterministic dynamics. This approach relies on a "cost-to-come value function that solves a Hamilton-Jacobi-Bellman (HJB) equation with Neumann boundary conditions in the viscosity sense.

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MS133

Duality of Nonlinear Filtering and Control

There is a fundamental dual relationship between estimation and control. The relationship compromises two concepts: (1) Duality between observability and controllability of a dynamical systems; (2) Duality between optimal filtering and optimal control. The interconnection of these two concepts is very well understood in linear-Gaussian settings. However for nonlinear problems, these two concepts have beed developed in isolation from each other. In this talk, the dual controllability problem for a hidden Markov model in continuous time is presented. The nonlinear filtering problem becomes an optimal control problem on the dual control system. The observability gramian is naturally defined from the duality theory. The proposed duality is shown to be an exact extension of the classical duality in linear systems theory. The duality is used to provide a sufficient condition for filter stability and the rate of convergence. A possible utility is to consider a sub-optimal control solution that leads to a novel algorithm for an approximation of the nonlinear filter.

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MS133

Particle-based Algorithm for Stochastic Optimal Control

The solution to a stochastic optimal control problem can be determined by computing the value function from a discretisation of the associated Hamilton-Jacobi-Bellman equation. Alternatively, the problem can be reformulated in terms of a pair of forward-backward SDEs, which makes Monte-Carlo techniques applicable. More recently, the problem has also been viewed from the perspective of forward and reverse time SDEs and their associated Fokker-Planck equations. This approach is closely related to techniques used in score generative models. Forward and reverse time formulations express the value function as the ratio of two probability density functions; one stemming from a forward McKean-Vlasov SDE and another one from a reverse McKean-Vlasov SDE. In this note, we extend this approach to a more general class of stochastic optimal control problems and combine it with ensemble Kalman filter type and diffusion map approximation techniques in order to obtain efficient and robust particle-based algorithms.

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MS134

High-Temperature Approximate Sampling for Surrogate Construction in Bayesian Inversion

Recent work [1, 2] uses approximate sampling methods such as the ensemble Kalman sampler (EKS) to find good interpolation points for constructing a surrogate model (using, e.g., Gaussian-process regression). Afterwards, an exact sampling method such as Markov chain Monte Carlo is employed to accurately sample from the (cheaper) surrogate. This can improve the sampling performance since it separates the two main tasks of a sampling algorithm: exploring the posterior distribution and producing samples from it. The former task is now executed by the approximate sampling method (which is used to construct the surrogate), whose evaluation points no longer need to sample from the posterior distribution. Motivated by the analytical work in [3], we study the effects of using in the above framework a high-temperature version of the distribution for the approximate sampler, producing extra samples from lower-probability regions. This can improve the exploration capabilities of the scheme, while the exact sampler can still sample from the correct distribution. [1] E. Cleary et al., "Calibrate, emulate, sample," J. Comput. Phys., 2021 [2] O. R. A. Dunbar et al., "Ensemble Inference Methods for Models With Noisy and Expensive Likelihoods," SIAM J. Appl. Dyn. Syst., 2022 [3] T. Helin et al., "Introduction To Gaussian Process Regression In Bayesian Inverse Problems, With New Results On Experimental Design For Weighted Error Measures." arXiv:2301.04518v2, 2023

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MS134

Neural Network Multi Fidelity Methods for Uncertainty Quantification in Kinetic Theory

In this talk, we will discuss the construction of novel multifidelity methods for kinetic equation where the low fidelity surrogates are composed by both simplfied macroscopic models and by neural network representation of the full model. Thanks to control variate approaches we show how these techniques are capable to reduce the variance of standard Monte Carlo techniques.

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MS134

Multilevel Monte Carlo Method uUsing the Parareal Algorithm

We are interested in approximating an expected value of a quantity of interest that arises from a stochastic differential equation using the parareal algorithm. For this estimation, Monte Carlo Method can be used. However, it can be computationally expensive particularly when it requires a computation with many timesteps. The Multilevel Monte Carlo method(MMC), introduced by Giles in 2008, is an approach that reduces the computational cost by performing most simulations with a low accuracy and corresponding low cost, and only very few simulations are performed at high accuracy and corresponding high cost. This is perfectly in line with the parareal algorithm that allows for different accuracies along the convergence process. In this talk, after recalling the basics of Multilevel Monte Carlo, we will explain how we can couple the MMC method with the parareal algorithm.

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MS135

Recent Advances in Consensus-Based Optimization

Consensus-based Optimization (CBO) is a particle method to solve global optimization problems which allows for a convergence proof on the level of the mean-field equation. In this talk we discuss the main characteristics of the method, the idea of the convergence proof and recent advances that concern different applications and problem classes. The theory is underpinned with numerical examples.

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MS136

Approximate Bayesian Computation for Model Calibration Given Summary Statistics

It is often the case in Bayesian parameter estimation that one has to contend with summary statistics on functions of the data on model observables, rather than having access to the data itself. For example, one may have access only to marginal moments on some quantity estimated from the data, but not the original data. In this setting, the challenge is to estimate a posterior density on model parameters given constraints on derived quantities. We have used maximum entropy and approximate Bayesian computation methods in this context to sample the joint space of data and parameters, accepting data sets consistent with available statistics, and employing opinion pooling methods to arrive at a pooled posterior on quantities of interest. We have applied this approach in multiple contexts, invoking approximations where necessary to tackle problem complexity. This talk will explore this landscape, and will highlight effective use of this construction in a recent study where we used summary information, in the form of nominal values and error bars, from multiple legacy experimental data sets, to arrive at a posterior on model parameters.

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MS136

Approximative Gaussian Likelihoods for Non-Gaussian Data

Despite all the advancements in the last decades, there are still many scenarios for which the standard inference techniques can't fully fulfil their purpose in identifying the distribution in the parameter space that describes a set of given measurements. In this talk, we present variations of the Bayesian synthetic likelihood approach that were revealed to be efficient in the parameter identification of non-Gaussian data while also being precise if applied to cases for which the theoretical posterior is well-known.

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MS136

Approximate Bayesian Computation for Probabilistic Damage Identification

Damage identification analyses are fundamental to guarantee the safety of civil structures. They are often formalised as inverse problems whose solution ignores any source of uncertainty that could be accounted for by using appropriate statistical models. Unfortunately, these models often exhibit an intractable likelihood function. We propose quantifying uncertainty through a fully Bayesian approach based on Approximate Bayesian Computation (ABC), a class of methods that overcome the likelihood evaluation and only require the ability to simulate from the model. Furthermore, we suggest a strategy to reduce the ABC computational burden using Neural Networks as surrogate models. Finally, we test the proposed method at work on a damaged beam to discuss its strengths and weaknesses.

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MS137

Adaptive Randomized Sketching for Dynamic Nonsmooth Optimization

Dynamic optimization problems arise in many applications, such as optimal flow control, full waveform inversion, and medical imaging. Despite their ubiquity, such problems are plagued by significant computational challenges. For example, memory is often a limiting factor when determining if a problem is tractable, since the evaluation of derivatives requires the entire state trajectory. Many applications additionally employ nonsmooth regularizers such as the L1-norm or the total variation, as well as auxiliary constraints on the optimization variables. We introduce a novel trust-region algorithm for minimizing the sum of a smooth, nonconvex function and a nonsmooth, convex function that addresses these two challenges. Our algorithm employs randomized sketching to store a compressed version of the state trajectory for use in derivative computations. By allowing the trust-region algorithm to adaptively learn the rank of the state sketch, we arrive at a provably convergent method with near optimal memory requirements. We demonstrate the efficacy of our method on a few control problems in dynamic PDE-constrained optimization.

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MS137

Randomized Approaches for OED

This work describe connections between optimal experiment design (OED) for PDE-based Bayesian linear inverse problems and the column subset selection problem (CSSP) in matrix approximation. We derive bounds, both lower and upper, for the D-optimality criterion via CSSP for the independent and coloured noise cases. Additionally, we describe ways to interpolate "left-out" sensor data using the "selected" sensors along with the errors in the data completion process. We develop and analyse randomised algorithms which achieve these bounds. Finally, we experimentally verify these results on a model advection-diffusion problem.

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MS137

Real-Time Uncertainty Quantification of Randomized Linear System Solvers

Randomized solvers for linear systems and least-squares problems can be deployed to speed up, or render feasible, the solution of such problems that arise inside of larger algorithms. However, these larger algorithms can only make use of such randomized subproblem solvers if they can have guarantees that the subproblem is sufficiently solved. Moreover, ensuring the subproblem's solution is sufficiently solved by a randomized procedure is not straightforward as traditional metrics of progress (e.g., a residual) cannot be practically calculated. Thus, even if a subproblem would be better solved by a randomized procedure, the outer algorithm may not be able to make use of this solution. In this talk, we will recast the tracking of a randomized solver's progress as a statistical hypothesis question, which we then solve by developing practical, real-time estimators for the solver's progress, and, more importantly, by developing practical, real-time uncertainty sets that allow us to control the false positive and false negative probabilities when answering the statistical hypothesis question. We will show that our tracking and uncertainty quantification methodologies are rigorous in theory, and practical in practice. We will conclude with some comments on how to integrate such information into larger algorithms, which we are actively working on to make rigorous.

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MS138

A Multi-Scale Deep Learning Framework for Projecting Weather Extremes

Extreme weather events are of growing concern for societies because under climate change, their frequency and intensity are expected to increase significantly. Unfortunately, general circulation models (GCMs)–currently the primary tool for climate projections–cannot characterize weather extremes accurately. Here, we report on advances

in the application of a multi-scale deep learning framework, trained on reanalysis data, to remedy deficiencies in GCMs to replicate the location, frequency, and intensity of tail events. The proposed approach 1) corrects the low-order and tail statistics of the GCM output at coarse scales; and 2) enhances the resolution of the debiased GCM output by reconstructing the finer scales as a function of the coarse scales. The novelty of our approach is to transform the GCM output without constraining the freedom of the climate model to sample the full distribution of possible extreme events consistent with near-present climate. This has significant implications for probabilistic risk assessment of natural disasters.

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MS138

First Steps Towards a Data-Driven Ensemble of Weather Forecasts

In recent years, there has been a rise in deep learning methods being used to produce highly accurate weather forecasts. So far, the leading approaches predict deterministic forecasts, but weather forecasting is inherently uncertain and understanding this uncertainty is vital, particularly for forecasting extreme events. In traditional numerical weather prediction, this uncertainty is normally quantified using an ensemble approach, where both the initial conditions and physical processes within the model itself are perturbed. How to quantify uncertainty for a data-driven forecast is non-trivial because it is not possible to simply perturb physical processes. This talk will therefore explore different approaches to create an ensemble of data-driven weather forecasts and show preliminary results using ECMWFs own data-driven model, AIFS.

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MS138

Modeling functional in(dependence) with neural networks

Given prior knowledge on the conditional independence structure of observed variables, often in the form of Bayesian networks or directed acyclic graphs, it is beneficial to directly encode such structure into neural networks during learning. This is particularly advantageous in tasks such as density estimation and generative modelling when data is scarce. We propose the Structured Neural Network (StrNN), which masks specific pathways in a neural network. The masks are designed via a novel relationship we explore between neural network architectures and binary matrix factorization, to ensure that the desired conditional independencies are respected and predefined objectives are explicitly optimized. We devise and study practical algorithms for this otherwise NP-hard design problem. We demonstrate the utility of StrNN in three applications: (1) binary and Gaussian density estimation with StrNN, (2) real-valued density estimation with Structured Autoregressive Flows (StrAFs), autoregressive normalizing flows that leverage StrNN as a conditioner, and (3) interventional and counterfactual analysis with StrAFs. Our work opens up new avenues for data-efficient generative modeling and the use of normalizing flows for causal effect estimation.

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MS138

A Probabilistic Framework for Using Data-assimilation and Machine Learning to Debias Under-resolved Climate Simulations

Accurately quantifying the risks of extreme weather events is becoming increasingly challenging due to our rapidly changing climate, yet it remains a critical step in the implementation of strategies to mitigate their impact on society. Due to the vast range of scales, simulating the fully turbulent climate system at full spatial resolution over any relevant time scale remains computationally out of reach. Therefore, we must rely on models which parametrize or completely ignore small-scale dynamics which can nontrivially affect the dynamics and statistics of the large-scale phenomena. In this work we present a probabilistic machine learning framework to correct under-resolved turbulent simulations to accurately reflect the fully resolved statistics. To overcome the challenge of chaotic divergence inherent in any turbulent system, we train our model on a coarse simulation nudged towards a high-resolution reference. This allows us to learn a correction operator which when evaluated on free-running coarse data – maps trajectories in the attractor of the coarse-scale system to ones in that of the fully-resolved system. Furthermore, we utilize architectures which inherently quantify the uncertainty in our predictions a critical function of any practical engineering tool. We illustrate our method on a prototypical turbulent climate model and show that our method is able to reconstruct the non-Gaussian statistics and characteristic features of the fully resolved data.

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MS139

Bridging the Gap Between Polar Observations and Modeling via Scientific Machine Learning

In this presentation, I will delve into the recent advancements we have achieved by harnessing the power of deep learning, encompassing both supervised and unsupervised classical techniques, as well as physics-informed deep learning approaches. At the heart of understanding glacier flow lies the challenge of comprehending the complex ice rheology governing these phenomena. Our ability to precisely predict global sea-level rise is limited by the sparse direct measurements of glacial ice properties which are not possible at a continental scale. Using physics-informed deep learning, we leverage the capabilities of back propagations to solve inverse problems, constrained by real-world satellite observations and the governing equations. I will demonstrate the importance of balancing the constraints of

physics, particularly in scenarios where data noise is prevalent. Our calculation yields discoveries of complex flow law of ice shelves that are different from commonly assumed forms, and suggests the need for reassessing the impact of our finding on the future projection of sea-level rise. Our results focus on the cryosphere, yet similar principles are applicable to problems involving data and governing equations, where deep learning is a promising method to accelerate scientific discoveries.

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MS139

Quantifying Uncertainty for Data-Driven Statistical Emulators of Climate

We introduce a data-driven approach to derive finite volume discretizations of a dynamical system's Continuity/Fokker-Planck equation, with a primary emphasis on quantifying uncertainty due to finite sample effects. Our method is extensible to function spaces and exhibits robustness against noise. Crucially, post-application, the methodology furnishes Markov states and a random matrix approximation to the generator, which, in tandem, mirrors the original system's statistics. We apply the method to a Held-Suarez atmospheric simulationa Flux-Differencing Discontinuous Galerkin discretization of the compressible Euler equations on a thin spherical shell. The technique effectively captures core statistical features like steady state moments, time autocorrelations, and residency durations in specific state space subsets.

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MS139

Physics-Infused Environmental Monitoring for Soil and Groundwater Contamination

Environmental monitoring traditionally relied on collecting point samples is undergoing transformational changes with new technologies such as remote sensing, in situ sensors and subsurface imaging. At the same time, environmental simulation capabilities are advancing rapidly, predicting complex flow and contaminant transport and quantifying its uncertainty. However, there are still significant challenges to integrate these multi-type multiscale datasets with model simulations. The Advanced Long-term Environmental Monitoring Systems (ALTEMIS) project aims to establish the new paradigm of long-term monitoring of soil and groundwater by integrating these new technologies through machine learning (ML). As a part of this framework, we have developed a Bayesian hierarchical approach coupled with non-stationary Gaussian process models to integrate in situ sensor data, groundwater sampling data and the ensemble simulations of the 3D groundwater and contaminant transport. The Bayesian approach provides a flexible framework to integrate the datasets with different accuracy and coverage and to propagate uncertainty. In addition, we defined the actual concentration as a function of simulated data within the Gaussian Process to accommodate the bias and errors in simulation results. This approach enables us to infuse physics such as the source location, flow direction and contaminant mobility into the spatiotemporal characterization of contaminant plumes.

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MS139

Uncertainty Quantification for Forward and Inverse Problems of PDEs via Latent Global Evolution

Deep learning-based surrogate models have demonstrated remarkable advantages over classical solvers in terms of speed, often achieving speedups of 10 to 1000 times over traditional partial differential equation (PDE) solvers. However, a significant challenge hindering their widespread adoption in both scientific and industrial domains is the lack of understanding about their prediction uncertainties, particularly in scenarios that involve critical decision making. To address this limitation, we propose a method that integrates efficient and precise uncertainty quantification into a deep learning-based surrogate model. Our method, termed Latent Evolution of PDEs with Uncertainty Quantification (LE-PDE-UQ), endows deep learning-based surrogate models with robust and efficient uncertainty quantification capabilities for both forward and inverse problems. LE-PDE-UQ leverages latent vectors within a latent space to evolve both the system's state and its corresponding uncertainty estimation. The latent vectors are decoded to provide predictions for the system's state as well as estimates of its uncertainty. In extensive experiments, we demonstrate the accurate uncertainty quantification performance of our approach, surpassing that of strong baselines including deep ensembles, Bayesian neural network layers, and dropout. Our method excels at propagating uncertainty over extended auto-regressive rollouts, making it suitable for scenarios involving long-term predictions.

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MS140

A Sampling Criterion for Constrained Bayesian Optimization with Uncertainties

We consider the problem of chance constrained optimization where it is sought to optimize a function and satisfy constraints, both of which are affected by uncertainties. The real world declinations of this problem are particularly challenging because of their inherent computational cost. To tackle such problems, we propose a new Bayesian optimization method. It applies to the situation where the uncertainty comes from some of the inputs, so that it becomes possible to define an acquisition criterion in the joint optimized-uncertain input space. The main contribution of this work is an acquisition criterion that accounts for both the average improvement in objective function and the constraint reliability. The criterion is derived following the Stepwise Uncertainty Reduction logic and its maximization provides both optimal design variables and uncertain parameters. Analytical expressions are given to efficiently calculate the criterion. Numerical studies on test functions are presented. It is found through experimental comparisons with alternative sampling criteria that the adequation between the sampling criterion and the problem contributes to the efficiency of the overall optimization.

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MS140

Adaptive Multi-Fidelity Monte Carlo for Realtime Storm Surge Hazard Quantification

Real-time, probabilistic predictions of the expected storm surge represent an important information source for guiding emergency response decisions during landfalling tropical storms. The uncertainty quantification in these predictions is accomplished as follows: an ensemble of probabilistic storm scenarios is generated; high-fidelity numerical simulations are performed to predict the surge for each of these scenarios; the simulation results are finally leveraged to estimate the statistics of interest. This process is repeated whenever a new storm advisory is issued. This paper investigates an adaptive Multi-Fidelity Monte Carlo (MFMC) framework for reducing the computational burden in the probabilistic estimation. As a lower-fidelity model within the MFMC setup, a surrogate model is adaptively developed based on high-fidelity numerical simulations from the current or past storm advisories. This accommodates a highly efficient information sharing across the hazard estimation for different advisories. To accommodate the use of high-fidelity simulations from the current advisory in the surrogate model calibration, the MFMC implementation is established using leave-one-out surrogate model predictions. Finally, the challenge of establishing MFMC predictions for a large number of quantities of interest (QoIs), corresponding to the surge at different geographic locations, is discussed.

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MS140

An Empirical Study of Gaussian Processes Learning in High Dimension: the Likelihood Versus Leave-One-Out Rivalry

Gaussian Process surrogates (GPs) are useful in the context of small data. However, GPs suffer particularly from the curse of dimensionality : at a fixed number of data points, their predictive capability may decrease dramatically in high dimension. In this talk, we investigate such a phenomenon in details. We illustrate this loss of performance with increasing dimension on simple functions and analyze its underlying symptoms, in particular a tendency to become constant away from the data points. We show that the fundamental problem is one of learning and not one of representation capacity: maximum likelihood, the dominant loss function for such models, can miss regions of optimality of the GP hyperparameters. Failure of maximum likelihood is related to statistical model inadequacy [F., Bachoc, Cross validation and maximum likelihood estimations of hyper-parameters of Gaussian processes with model misspecification, Comput. Stat. & Data Analysis, 2013] : a model with constant trend is sensitive to dimensionality when fitting quadratic functions while it much better handles dimension growth for linear functions or Gaussian trajectories generated with the right covariance. Our experiments also show that the leave-one-out loss function is less prone to the curse of dimensionality even for inadequate statistical models.

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MS141

Theoretical Analysis of the Resampled Ensemble Kalman Filter

Filtering is concerned with online estimation of the state of a dynamical system from partial and noisy observations. In applications where the state of the system is high dimensional, ensemble Kalman filters are often the method of choice. These algorithms rely on an ensemble of interacting particles to sequentially estimate the state as new observations become available. Despite the practical success of ensemble Kalman filters, theoretical understanding is hindered by the intricate dependence structure of the interacting particles. This talk will discuss ensemble Kalman filters that incorporate an additional resampling step to break the dependency between particles. The new algorithm is amenable to a non-asymptotic and dimension-free theoretical analysis that extends and improves upon those available for filters without resampling, while also performing well in numerical examples.

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MS141

Improving Enkf Performance By Adaptively Controlling The Ensemble

Efficient strategies to improve the performance of the Ensemble Kalman Inversion by adaptively controlling the ensemble. Due to their low computational costs and straightforward implementation, filtering methods such as the Ensemble Kalman Filter have become very popular for inverse

problems over the last few years.They have been demonstrated to work well even for highly nonlinear, complex models. We discuss variants of the Ensemble Kalman Inversion (EKI) aiming to improve the accuracy of the estimate by adaptively choosing the particles in the ensemble.

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MS141

Blending Ensemble Kalman and Diffusion Models, from the Bayesian Sampling Perspective

Sampling, at large, is to draw a sample from a target distribution. The distribution can be given by its mathematical from, $\rho(x) \propto \exp(-f(x))$ with the accessing to the evalutations of $f(x)$. Or can be given by many of its representative samples $\{x_i\}_{i=1}^N \sim \rho$. Ensemble Kalman methods, like many other Bayesian sampling method, is to find i.i.d. samples from the given form using the information about f. While diffusion model is to generate new samples based on the N existing samples that represent the underlying distribution. Suppose we both have some existing representative samples, and have the access to the potential $f(x)$, can we integrate the ensemble methods and the diffusion model to improve the sampling quality of Ensemble Kalman methods? We give an initial attempt at this problem. In particular, we use samples generated by Ensemble Kalman methods as the base samples to build up the diffusion model. This not only recycles the information achieved by Ensemble Kalman methods, but also integrate the theoretical guarantee provided by the diffusion models. We show that our method provides an accurate sampling strategy for distributions that are not log-concave both theoretically and numerically.

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MS141

High Dimensional Ensemble Kalman Inversion with Localization

Ensemble Kalman inversion (EKI) is a technique for the numerical solution of inverse problems. A great advantage of the EKI's ensemble approach is that derivatives are not required in its implementation. But theoretically speaking, EKI's ensemble size needs to surpass the dimension of the problem. This is because of EKI's "subspace property", i.e., that the EKI solution is a linear combination of the initial ensemble it starts off with. We show that the ensemble can break out of this initial subspace when "localization" is applied. In essence, localization enforces an assumed correlation structure onto the problem, and is heavily used in ensemble Kalman filtering and data assimilation. We describe and analyze how to apply localization to the EKI, and how localization helps the EKI ensemble break out of the initial subspace. Specifically, we show that the localized EKI (LEKI) ensemble will collapse to a single point (as intended) and that the LEKI ensemble mean will converge to the global optimum at a sublinear rate. Under strict assumptions on the localization procedure and observation process, we further show that the data misfit decays uniformly. We illustrate our ideas and theoretical developments with numerical examples with simplified toy problems, a Lorenz model, and an inversion of electromagnetic data, where some of our mathematical assumptions may only be approximately valid.

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MS142

Bayesian Shape Inversion for Scattering Transmission Problems

In the field of nano-optics, one works with very small objects, which cannot be made in the exact shape intended due to the manufacturing process. Therefore, it is useful to know how these objects deviate from their intended shape to better predict their experimental behaviour. This can be determined from experimental measurements using Bayesian inversion and assuming that the involved wave obeys the Helmholtz equation. We prove that the resulting inverse problem is well-posedness in a wave number-explicit way. To solve the forward problem numerically, finite elements are used as well as a mapping approach to a reference configuration to handle the sample-dependent geometry and a perfectly matched layer to approximate the radiation condition at infinity. The posterior distribution is approximated using sequential Monte Carlo with adaptive tempering. We will show numerical results to demonstrate the feasibility and potentiality of this approach as well as the effect of the frequency on the posterior concentration.

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MS142

Parametric PDE Solvers in Parametric Domains

Solving parametric Partial Differential Equations (PDEs) in parametric domains is a challenging problem from a computational point of view. It is a first step towards taking into account the uncertainty in the domain and how it affects the solution, in view of performing data assimilation, control and optimisation. First, we will present a non-linear manifold reduction method to parsimoniously represent parametric characteristic functions of sets. The method is constructive and rely on introducing a ridge regression exploiting linear information on the characteristic functions. Some analysis results and numerical experiments will be shown. In particular, we will see how the

method is able to overcome the so-called Kolmogorov barrier for some classes of meaningful parametric characteristic functions. Second, we will show how this representation of the characteristic functions can be used in order to efficiently compute the solution of parametric PDEs in uncertain domains. A non-linear way to represent the solution is introduced, making it possible to have some guarantees in terms of accuracy. We will show several numerical experiments to illustrate the properties of the methods.

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MS142

Reduced Order Methods for UQ in Domains with Parametric Geometries

We do provide the state of the art of our work on reduced order methods dealing with bifurcations in parametric systems held by stochastic nonlinear PDEs. Domains by Parametric geometries are a natural field of application for reduced order methods.

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MS143

Computing Capacitance Using Alpha-Stable Sample Paths

A method is described for computing alpha-capacity of sets in d-dimensions through the use of simulated continuous time process with isometric stable increments. A method we call Walk-In-Out-Balls is described to simulate points from the equilibrium measure of a set. These points are then used to estimate the Riesz capacity of the set.

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MS144

Fully Personalised Degenerative Disease Modelling a Duchenne Muscular Dystrophy Case Study

The ambulatory abilities of Duchenne Muscular Dystrophy (DMD) patients can be measured using the NSAA score. This test can be taken many times, giving a trajectory over time. The ability to extrapolate these trajectories effectively would give clinicians the opportunity to construct treatment plans earlier, allowing treatments to be taken in advance of worsening of conditions. Furthermore, the data-sets available have high missingness, and the creation of a model for DMD progression provides an opportunity for high quality synthetic data without missingness to be constructed. Therefore, we create a hierarchical Bayesian model for NSAA scores, allowing personalised, probabilistic trajectory predictions to be made. Variations of this model can be created, such as the way discrepancy is modelled, if we should covary parameters with other predictors, and whether to include terms for treatments. We hence examine criterion such as quantile coverage, sharpness, and the quality of synthetic data to perform model selection. Additionally, we try to determine how effective the model is at predicting minimal clinically important differences, in order to determine if the predictions made can be clinically useful.

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MS144

Uncertainty and Sensitivity Analysis for Real-World Problems in Clinical Cardiology

Clinical medicine increasingly makes use of high resolution imaging and sophisticated physiological measurement for diagnosis and to guide interventions. In the case of the heart and cardiovascular system, some physiological parameters (for example heart rate and ejection fraction) can be accessed easily through imaging and measurement, but others (for example electrical activation and recovery within the tissue) are either hard or impossible to measure in a patient. There is an increasing desire to use models of structure and function to both infer parameters that are difficult to measure and to predict the outcome of an intervention. Clinical data are frequently noisy and incomplete, and so these approaches need to take into account uncertain inputs, and to propagate uncertainty through to outputs and predictions. This talk will focus on the use of probabilistic and patient-specific models of the human left atrium, and how these can be used to predict the outcome of treatments for atrial fibrillation.

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MS144

Uncertainty Quantification in a Cardiac Arrhythmia Model: Application to IntraAtrial Reentrant

Tachycardia (IART)

Cardiac Arrhythmia are a leading cause of death according to the WHO statistics. To support clinical practice and lower mortality, Cardiac Digital Twins are developed to assess the origin of arrhythmias and non-invasively test treatments, leading to patient specific medicine. This involves the selection of an appropriate model to describe the heart and its diseased tissue, after which the model parameters can be inferred from personalized data. However, it is important to assess the uncertainty on the inferred parameters as well, in order to make well-motivated clinical decisions. In this talk, a forward model to describe the specific case of IntraAtrial Reentrant Tachycardia (IART) is shown. This is an arrhythmia in which a non-linear excitation wave is attached to an anatomical obstacle, mostly resulting from earlier surgery. The shape, position, and orientation of the scar in a 2D model are important characteristics for the evolution of the pathological excitation wave. To serve as realistic input for a Markov Chain Monte Carlo (MCMC) Bayesian inversion algorithm, synthetic cardiac electrogram data is generated from computer simulations. Results and the feasibility of this approach in terms of accuracy and computation time are shown.

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MS144

Non-Implausible Set Detection via Branching Subset Simulation

History matching aims at identifying a subset of a model's input space which results in an output that is likely to match an observation or target, all sources of uncertainty considered. This set, referred to as the non-implausible domain, can be orders of magnitude smaller than the original input space. It can also be high-dimensional and disconnected, for which sampling from it is very challenging. Recently, a solution based on generating rare events using Subset Simulation was proposed. The solution is robust to high dimensionality, but cannot always guarantee that it will explore the whole input space, therefore missing disconnected subsets of the non-implausible set and producing bias. We present Branching Subset Simulation, an algorithm that partitions the input space recursively, and where each partition (called a branch) starts Subset Simulation anew. We demonstrate that this results in a more comprehensive exploration of the input space and that the same paradigm can be used not only for calibration but for reliability analysis and optimisation.

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MS145

Computational Hypergraph Discovery

Most scientific challenges can be framed into one of the following three levels of complexity of function approximation. Type 1: Approximate an unknown function given input/output data. Type 2: Consider a collection of variables and functions, some of which are unknown, indexed by the nodes and hyperedges of a hypergraph (a generalized graph where edges can connect more than two vertices). Given partial observations of the variables of the hypergraph, approximate all unknown functions. Type 3: if the hypergraph structure itself is unknown, use partial observations of the variables of the hypergraph to discover its structure and approximate its unknown functions. While most Computational Science and Engineering challenges can be framed as Type 1 and 2 problems, many scientific problems can only be categorized as Type 3. Despite their prevalence, these Type 3 challenges have been largely overlooked due to their inherent complexity. We introduce an interpretable GP framework for Type 3 problems, targeting the data-driven discovery and completion of computational hypergraphs. Our approach is based on a kernel generalization of (1) Row Echelon Form reduction from linear systems to nonlinear ones, (2) variance-based analysis. Here, variables are linked via GPs, and those contributing to the highest data variance unveil the hypergraphs structure. We illustrate the proposed approach with applications to equation discovery, network discovery, and raw data analysis.

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MS145

Optimal Krylov on Average

Krylov subspace methods are frequently employed as linear system solvers in the inner loop of Gaussian process (GP) training. However, the deterministic early truncated version introduces bias into the solution, leading to underfitting. Previous works in constructing randomized truncation estimators for conjugate gradients (CG) render the GP training unbiased at the cost of introducing variance. These methods determine the truncation distribution beforehand based on the exponential error estimates of CG, which lose CG's adaptivity to a wide range of linear systems. This work introduces an adaptive truncation estimator, applicable to CG and minimal residual methods, that optimizes the trade-off between the variance and the computation cost. We construct a constraint optimization problem and compute the truncation probabilities throughout the iterations. We derive an optimal closed-form solution when the improvement of the deterministic algorithm satisfies a diminishing returns property. We prove that obtaining the optimal adaptive truncation distribution is impossible in the general case. Without the diminishing returns condition, our estimator provides a suboptimal but still unbiased solution. We present experimental results in GP hyperparameter tuning to demonstrate the effective-

ness of our approach.

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MS145

Numerical Methods for Scalable Gaussian Processes and Beyond

no text at time

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MS146

Monte Carlo Is a Good Sampling Strategy for Polynomial Approximation in High Dimensions

When approximating of smooth, high-dimensional functions from limited samples using polynomials it is common to use Monte Carlo sampling, so as not to succumb to the curse of dimensionality. However, it is well known that such a strategy is theoretically suboptimal. Specifically, there are many polynomial spaces of dimension n for which the sample complexity scales log-quadratically, i.e., like $c \cdot n^2 \cdot \log(n)$ as $n \to \infty$. This well-documented phenomenon has led to a concerted effort over the last decade to design improved, and moreover, near-optimal strategies, whose sample complexities scale log-linearly, or even linearly in n. In this work we demonstrate that Monte Carlo is actually a perfectly good strategy in high dimensions, despite its apparent suboptimality. We first document this phenomenon empirically via a systematic set of numerical experiments. Next, we present a theoretical analysis that rigorously justifies this fact in the case of holomorphic functions of infinitely-many variables. Overall, our findings suggest that Monte Carlo sampling is a good choice for polynomial approximation in high dimensions and shed light on why this is the case. Therefore, the benefits of improved sampling strategies are generically limited to lower-dimensional settings.

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MS146

Sample-Efficient Techniques for Deep Learning of High-Dimensional Banach-Valued Functions

Reconstructing high-dimensional functions from limited samples is a central challenge in uncertainty quantification for computational science and engineering. Approaches based on deep learning have achieved impressive results in modeling such problems, which are often stated in terms of parameterized partial differential equations or operators mapping functions or parameters to infinite-dimensional Hilbert or Banach spaces. In this study, we present an innovative algorithmic approach that incorporates deep learning, compressed sensing, orthogonal polynomials, and finite elements to approximate smooth functions taking values in such spaces. Our theoretical analysis provides explicit guarantees on error and sample complexity in solving such problems. We complement this with numerical experiments demonstrating accurate approximations on challenging benchmark problems. Furthermore, we show how recent active learning techniques based on Christoffel sampling can lead to significant savings in the number of samples.

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MS146

The Role of Statistical Theory in Understanding Deep Learning

In recent years, there has been a surge of interest across different research areas to improve the theoretical understanding of deep learning. A very promising approach is the statistical one, which interprets deep learning as a nonlinear or nonparametric generalization of existing statistical models. For instance, a simple fully connected neural network is equivalent to a recursive generalized linear model with a hierarchical structure. Given this connection, many papers in recent years derived convergence rates of neural networks in a nonparametric regression or classification setting. Nevertheless, phenomena like overparameterization seem to contradict the statistical principle of bias-variance trade-off. Therefore, deep learning cannot only be explained by existing techniques of mathematical statistics but also requires a radical overthinking. In this talk we will explore both, the importance of statistics for the understanding of deep learning, as well as its limitations, i.e., the necessity to connect with other research areas.

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MS146

Analysis of Vector-Valued Random Features

This talk provides a complete error analysis of learning with vector-valued random features (RF). The theory is developed for RF ridge regression in a fully general infinite-dimensional input-output setting, but nonetheless applies to and improves existing finite-dimensional analyses. In contrast to comparable work, the approach proposed here relies on a direct analysis of the underlying risk functional and completely avoids the explicit RF ridge regression solution formula in terms of random matrices. This removes the need for concentration results in random matrix theory. The main results established in this paper include

strong consistency of RF estimators under model misspecification and explicit convergence rates in various settings. The number of random features and number of labeled data required to achieve such rates are comparable with Monte Carlo intuition and free from logarithmic factors for the first time.

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MS147

Scalable Analytical Inference for Bayesian Deep Learning

Neural networks trained with gradient descent (i.e., backprop) have a limited capacity to quantify the epistemic uncertainties associated with their parameters along with the aleatory uncertainties associated with their predictions. Several approximate methods have been proposed to apply Bayesian inference in neural networks, yet none of them has displaced deterministic gradient-based training in mainstream applications. This contribution will present the new Tractable Approximate Gaussian Inference (TAGI) method that has the potential to bring a paradigm shift by enabling analytical inference in deep neural networks. We will cover the fundamentals behind the TAGI method, along with a review of the specific structure and connectivity of neural networks which justify the assumptions and approximations made. TAGI's performance will be benchmarked against other methods for a variety of tasks ranging from small regression problems, to deep architectures with 10M+ parameters applied on classification, reinforcement learning, and time-series problems. We will show how unlocking the capacity to perform analytical Bayesian inference in large neural networks allows for unprecedented applications and possibilities.

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MS147

How to Build Machines that Adapt Quickly

Humans and animals have a natural ability to autonomously learn and quickly adapt to their surroundings. How can we design machines that do the same? In this talk, I will present Bayesian principles to bridge such gaps between humans and machines. I will discuss (1) the Bayesian learning rule to unify algorithms; (2) sensitivity analysis to understand and improve memory of the algorithms; and (3) new priors to enable quick adaptation. These ideas are unified in a new learning principle called the Bayes-duality principle, yielding new mechanisms for knowledge transfer in learning machines. References: - The Bayesian Learning Rule, (JMLR 2023) M.E. Khan, H. Rue - The Memory Perturbation Equation: Understanding Models Sensitivity to Data, (NeurIPS 2023) P. Nickl, L. Xu, D. Tailor, T. Mllenhoff, M.E. Khan - Knowledge-Adaptation Priors, (NeurIPS 2021) M.E. Khan, S. Swaroop - Continual Deep Learning by Functional Regularisation of Memorable Past (NeurIPS 2020), P. Pan, S. Swaroop, A. Immer, R. Eschenhagen, R. E. Turner, M.E. Khan

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MS147

Stochastic Gradient Descent, a Scalable Algorithm for Gaussian Processes and Linear Models

Bayesian neural networks and Gaussian Processes are some of the most powerful and performant techniques that exist for principled uncertainty estimation, but they have remained impossible to scale due to cubic scaling dependencies in either the number of datapoints or number of parameters. In this talk, drawing on ideas from sampling-based inference and pathwise conditioning, we propose stochastic gradient algorithms that can scale posterior inference in BNNs and GPs to millions of datapoints (Imagenet-1000 and 2.5 million dimensional UCI datasets) and millions of parameters (ResNet-50 and 3D UNet models). We show interesting results through a spectral characterization of the implicit bias of stochastic gradient descent, and show that it produces predictive distributions close to the true posterior both in regions with sufficient data coverage, and in regions sufficiently far away from the data. Using our proposed approach, we obtain high-quality uncertainty estimates that can enable strong downstream applications such as Thompson sampling and experimental design.

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MS147

Uncertainty Quantification in Reinforcement Learning

We consider the problem of quantifying uncertainty over expected cumulative rewards in model-based reinforcement learning. In particular, we focus on characterizing the variance over values induced by a distribution over MDPs. Previous work upper bounds the posterior variance over values by solving a so-called uncertainty Bellman equation, but the over-approximation may result in inefficient exploration. We propose a new uncertainty Bellman equation whose solution converges to the true posterior variance over values and explicitly characterizes the gap in previous work. Moreover, our uncertainty quantification technique is easily integrated into common exploration strategies and scales naturally beyond the tabular setting by using standard deep reinforcement learning architectures. Experiments in difficult exploration tasks, both in tabular and continuous control settings, show that our sharper uncertainty estimates improve sample-efficiency.

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MS148

On the Asymptotic Efficiency of Adaptive Multilevel Splitting in the Small Noise Regime

The AMS algorithm is a Monte Carlo method that is now well established to sample rare events by iteratively simulating clones of the process and selecting trajectories that have reached the highest value of a so-called importance function. In this talk, the large sample size relative variance of the AMS small probability estimator will be considered. The main result is a large deviations logarithmic equivalent of the latter in the small noise asymptotics, which is rigorously derived. It is given as a maximisation problem explicit in terms of the quasi-potential cost function associated with the underlying small noise large deviations. A simple geometric condition ensuring a property of weak asymptotic efficiency will be presented: each level set of the importance function must contain a state which minimizes simultaneously i) the quasi-potential cost function from the initial condition, and ii) to the target rare event. Time permitting, interpretations and practical consequences will be discussed. This is a joint work with Mathias Rousset and Sofiane Martel.

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MS148

An Energy-based Model Approach to Rare Event Probability Estimation

Rare event probability estimation often encompasses determining the probability of a hazard or system failure occurring when a quantity of interest exceeds a critical value. In our approach, we represent the distribution of the quantity of interest using an energy density, defined by a free energy function, and enhance the estimation of the free energy by introducing a bias potential. Leveraging concepts from energy-based models (EBM), this bias potential is optimized such that the corresponding probability density function approximates a pre-defined distribution targeting the failure region of interest. Once the optimal bias potential is determined, we can calculate the free energy function and the rare event probability of interest. To strike a balance between accuracy and efficiency, we incorporate a stopping criterion based on the Stein discrepancy into the EBM approach. Furthermore, we investigate both parametric and non-parametric techniques for the bias potential, with the latter eliminating the need for specific parameterization but relying heavily on the kernel density estimate used in the optimization process. By presenting illustrative test cases that encompass both traditional and inversion scenarios, we showcase that our suggested EBM approach, when configured appropriately, enables stable and efficient estimation of rare event probabilities and compares favorable against subset sampling methods.

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MS148

Neural Networks Based Learning Applied to Extreme Statistics and Sampling Rare Events

Feedforward neural networks based on Rectified linear units (ReLU) cannot efficiently approximate quantile functions which are not bounded, especially in the case of heavy-tailed distributions. This is a major issue for any use in quantile approximation or sampling scheme (such as generative modelling). In this talk we design and compare several new parametrizations for the quantiles (and for the generator of a Generative adversarial network) adapted to this framework, basing on extreme-value theory. We provide theoretical convergence results (as the complexity of the NN increases) and we illustrate the resulting methodologies with experimentations on both simulated data and real data.

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MS148

Importance Sampling for Rare Events and Some Pathologies of the Exit Problem

Importance sampling and multilevel splitting are key techniques for rare event simulation. Yet they may produce poor results or become inefficient for bad choices of a proposal distribution (in case of importance sampling) or an inappropriate design of the intermediate checkpoints or milestones (in case of multilevel splitting). The problem is known to be more severe for importance sampling, since the likelihood ratio that appears in the importance sampling estimator is not bounded a priori (in contrast to the particle weights in splitting), which may render importance

sampling estimators useless in certain situations, especially for systems with high-dimensional state space or for processes involving long trajectories. We discuss importance sampling of exit problems that involve unbounded stopping times; examples are mean first passage times, transition rates or committor probabilities in molecular dynamics. The naive application of variance minimization techniques can lead to pathologies here, including proposals measures that are not absolutely continuous to the reference measure or importance sampling estimators that formally have zero variance, but that produce infnitely long trajectories. In this presentation, we will illustrate these issues with simple examples and discuss possible solutions that are based on a risk-sensitive optimal control framework of importance sampling.

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MS149

ParticleDA.jl v.1.0: A Distributed Particle Filtering Data Assimilation Package

Digital twins of physical and human systems informed by real-time data, are becoming ubiquitous across weather forecasting, disaster preparedness, and urban planning, but researchers lack the tools to run these models effectively and efficiently, limiting progress. One of the current challenges is to assimilate observations in highly non-linear dynamical systems, as the practical need is often to detect abrupt changes. We have developed a software platform to improve the use of real-time data in non-linear system representations where non-Gaussianity limits the applicability of data assimilation algorithms such as the ensemble Kalman filter and variational methods. Particle filter based data assimilation algorithms have been implemented within a user-friendly open source software platform in Julia - ParticleDA.jl. To ensure the applicability of the developed platform in realistic scenarios, emphasis has been placed on numerical efficiency and scalability on high performance computing systems. Furthermore, the platform has been developed to be forward model agnostic, ensuring that it is applicable to a wide range of modelling settings, for instance unstructured and non-uniform meshes in the spatial domain or even state spaces that are not spatially organized. Applications to tsunami and numerical weather prediction demonstrate the computational benefits and ease of using the high-level Julia interface to the package to perform filtering in a variety of complex models.

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MS149

Enhancing Bayesian Model Updating in Structural Health Monitoring via Learnable Mappings

We present a new way to enhance stochastic approaches to structural health monitoring through the use of a learnable feature extractor and a feature-oriented surrogate model, both based on deep neural networks. These two data-driven models work in tandem to evaluate a likelihood function within a Markov chain Monte Carlo sampling algorithm. The feature extractor maps sensor recordings onto a low-dimensional metric space that encapsulates the sensitivity to structural health parameters. On the other hand, the surrogate model maps the structural health parameters onto their feature description. The procedure enables the updating of beliefs about the structural health parameters, effectively replacing the need for a computationally expensive finite element model. During a preliminary offline phase, we generate a labeled dataset to train both the feature extractor and the surrogate model. Within a simulation-based framework, training vibration responses are efficiently generated by means of a multi-fidelity surrogate modeling strategy. This multi-fidelity strategy exploits model order reduction and deep learning to speed up the data generation phase while preserving the damage-sensitivity of the approximated signals. The proposed strategy is assessed through synthetic test cases, demonstrating impressive results in terms of accuracy of the estimated quantities and computational efficiency.

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MS149

Goal-oriented Projection-Based MOR for Inverse Problems

The use of surrogate modeling techniques for estimating the state of systems described by parameterized partial differential equations has been of great interest in recent years in the data assimilation community. The parameter associated with the observed state is also usually of great interest, e.g. in optimal control problems. Ideally, the introduction of a surrogate model should reduce the computational cost, particularly in comparison to the Full Order Model (FOM), while introducing the minimal possible approximation error. In particular, surrogate models based on standard estimation techniques such as the least-squares or Galerkin method introduce approximation errors on the predicted observations. Reducing such errors ensures that the results of the data assimilation will be closer to obtained using the FOM. In our work, we propose to build a reduced order model that minimises the error on the predicted observations. This method is can be viewed as an angled proper orthogonal decomposition method since it implies a modification of the inner product used in the computation of the snapshot correlation matrix. A challenge associated to the method we propose is to correctly exploit the newly produced reduced space, in order to preserve its properties with respect to observation operator, while using it for estimation. We propose techniques to address this current limitation, and thus, enhancing estimations keeping a negligible computational cost.

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MS149

Balanced Truncation for Ensemble Kalman Inversion

The Ensemble Kalman filter is a classical method for solving data assimilation problems in which a stream of incoming data is used to update the underlying state of a model sequentially in time. The Ensemble Kalman Inversion (EKI) approach re-interprets the ensemble Kalman filter as a method for solving more general inverse problems. For high-dimensional smoothing problems (where the state to be inferred is the unknown initial condition and the indirect measurements are taken at times $t > 0$), a high-dimensional ODE must be solved for each particle at each iteration of the EKI approach. Because the EKI error scales at the Monte Carlo rate $N^{-\frac{1}{2}}$ (where N is the number of particles in the ensemble), this cost can be prohibitive. Balanced truncation for Bayesian inference (BTBI) is a recently introduced model reduction method for linear dynamical systems tailored to the Bayesian smoothing problem. This talk will introduce EKI and BTBI and describe how their union leads to efficient solution of the smoothing problem.

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MS150

Nonlinear Forces and Omitted Masses: Mass-Spring-Damper Models and Their Model-Form Errors

In structural dynamics, gathering high-fidelity observations is often prohibitively expensive, and low-fidelity mass-spring-damper models generate predictions and inform decisions, such as defining a bridge's maximum load, chronicling the dynamics of a jointed structure, or describing a driving cars vertical behavior. But significant discrepancies between observations and predictions often result from model-form error (MFE) (e.g., missing dependencies or simplified forces). Therefore, we investigate MFE in low-fidelity linear models, specifically in damping and spring forces, and with observations from several systems—linear high-fidelity models, nonlinear high-fidelity models, and experiments. We embed an enrichment operator into the low-fidelity model to form an enriched model which retains the low-fidelity state variables, reduces discrepancies, and allows for extrapolative predictions. Results show excellent agreement between enriched model predictions and observations from linear systems. We analyze when the enriched model is able to reduce discrepancies caused by nonlinear forces and circumstances in which the enriched model fails.

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MS150

Challenges in Model-Form Uncertainty Quantification Using Experimental Data From a Vibration Isolation Example

This contribution gives a comprehensive background of Bayesian statistics from the bottom up with an engineering application example. Probability theory using set theory and Venn diagrams illustrate the roots of the Bayesian equation in its basic form. It includes the background and meaning of the essential elements: the prior probability of a hypothetical event, the likelihood of a symptomatic event under the condition that the hypothetical event already happened, the total probability of the symptomatic event, and the posterior probability of the hypothetical event under the condition that the symptomatic event already happened. The Bayesian approach is the framework to estimate the uncertainty of two different analytical model forms used to predict the passive and active vibration isolation behavior for an oscillating mass. In this context, active vibration isolation means that additional controlled forces change and adapt the damping properties to enhance the vibration isolation behavior. Passive vibration isolation is without the additional controlled forces. The first model form describes the oscillating mass as part of a simple one-mass oscillator; the second model form uses the oscillating mass as part of a simple two-mass oscillator. Both model forms contain assumptions about inertia, damping, and stiffness properties representing hypothetical events. Experimental vibrational data measured from a realized test setup serves as the symptomatic outcome or event.

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MS150

Assessing Model Prediction Trustworthiness in the Presence of Model-Form Uncertainty

In the process of model development, limited knowledge and computational resources necessitate simplifying assumptions that are not valid in all cases, leading to model-form uncertainty. Understanding the impact these assumptions (and their uncertainties) have on model predictions is critical to judging the reliability of the predictions to inform high-consequence engineering-design and policy decisions. We present a novel method to quantify this impact by combining parameterized perturbations to modeling assumptions with grouped variance-based sensitivity analysis. Additionally, we demonstrate how the method can be used to measure whether an assumption has been stress-tested during validation, based on whether it was impor-

tant to model outputs both in the prediction scenario and the validation scenario.

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MS151

Efficient PDE-Constrained Optimization Using Derivative-Informed Neural Operators

We present a novel framework for solving PDE-constrained optimization problems under uncertainty (OUU) problems using derivative-informed neural operators (DINOs). OUU problems are often orders of magnitude more expensive to solve compared to their deterministic counterparts because of the evaluation of the statistical/risk measures by stochastic integration. To tackle this computational challenge, we propose the use of a multi-input reduced-basis network to approximate the PDE mapping from the input spaces of the uncertain parameter and the optimization variable to the output state. In particular, we incorporate derivatives of the PDE operator into a Sobolev-type training loss to ensure that the neural operator has accurate derivatives with respect to the optimization variable due to its importance in for the derivative-based optimization of the OUU objective. We demonstrate the performance of our method over a suite of numerical experiments, showcasing the accuracy and sample efficiency of the DINOs in the solving the OUU problems.

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MS151

Multidimensional Quadrature Rule for Integrals with Exotic Weights

The classical weighted quadrature rules rely on roots of orthogonal polynomial and work well in context when the roots are well defined and real, e.g., in the case when the weight function is positive definite. In this work, we present a method for quadrature construction that extends to the setting where the weight function is negative but bounded from below. The asymptotic convergence rate of our method trails that of the classical Gauss-Legendre quadrature. However, in the pre-asymptotic regime our exotic construction vastly outperforms the classical approach and is further magnified when applied in a multi-dimensional context, such as many application of (Uncertainty Quantification and radiation transport).

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MS152

Trajectory-Oriented Optimization of Stochastic Epidemiological Models

Epidemiological models must be calibrated to ground truth for downstream tasks such as producing forward projections or running what-if scenarios. The meaning of calibration changes in case of a stochastic model since output from such a model is generally described via an ensemble or a distribution. Each member of the ensemble is usually mapped to a random number seed (explicitly or implicitly). With the goal of finding not only the input parameter settings but also the random seeds that are consistent with the ground truth, we propose a class of Gaussian process (GP) surrogates along with an optimization strategy based on Thompson sampling. This Trajectory Oriented Optimization (TOO) approach produces actual trajectories close to the empirical observations instead of a set of parameter settings where only the mean simulation behavior matches with the ground truth

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MS152

Learning-Based Estimation and Uncertainty Quantification of Nonlinear Inverse Operators

Recent advances in deep operator learning have provided networks capable of yielding flexible, accurate, data-driven models of complex systems. However, regardless of precision, these models are still idealizations of reality; and hence, demand quantification and aid in reducing uncertainties. This presentation explores the use of conformal prediction (whose attractive qualities include non-asymptotic coverage guarantees as well as demanding the most limited of model assumptions) to quantify functional outcome uncertainties in the form of non-parametric quantile regression. To help showcase these methods (and compare other learning architectures) we employ the well-known and accessible remote sensing atmospheric data available through NASAs OCO-2 carbon dioxide measurement mission

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MS152

Reinforcement Learning for the Adaptive Construction of Surrogate Models

The computational costs of high-fidelity numerical models often limit the number of model queries that can be made in practice. For outer-loop analysis tasks, such as uncertainty quantification and inverse problems, this poses a key practical challenge since most algorithms will fail to converge when insufficient model evaluations are available. To overcome this, surrogate models are increasingly being used to drive research and development efforts. These models provide lightweight approximations to the full models and can be queried more efficiently to facilitate outer-loop analysis. However, this approach is only effective when the surrogate models are accurate representations of the original models. Since the number of model queries is still limited, the surrogates must be constructed using carefully selected queries that reveal as much information as possible. In this talk, we discuss the potential for using reinforcement learning to create adaptive sampling strategies tailored to specific surrogate use-cases. We consider a collection of distinct quantities of interest, and task reinforcement learning agents with proposing query locations that result in the most accurate surrogate models. We show that these agents identify distinct strategies for each quantity of interest by learning how to position queries most effectively based on the task at hand

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MS153

Learning Distributions with Regularized JKO Scheme and Low-Rank Tensor Decompositions

The theory of Wasserstein gradient flows gives a framework for sequentially constructing approximations to complicated distributions, which may arise from applications such as Bayesian inversion, importance sampling and generative modelling. For high dimensional problems, Eulearian methods are not usually used, because in general, they suffer from the curse of dimensionality. In the current talk, we attempt to "rehabilitate" the Eulerian methods in high dimension by using the developments in low-rank Tensor Train decomposition. The approach is based on the Fisher Information regularization of the dynamic JKO scheme. This essentially is a proximal step with respect to the Wasserstein distance and can be viewed as a generalization of the implicit gradient descent method. The nonlinear transformation of variables allows to represent the problem as a system of heat equations with nonlinear coupling in the initial and terminal condition. The system is formulated as a fixed-point equation, and we explore the possibility of solving it with accelerated methods. An ODE governing the evolution of particles can be defined with help of intermediate variables, giving a deterministic sampling algorithm for the approxinate distribution.

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MS153

Solving Nonlinear Filtering Problems Using a Tensor Train Decomposition Method

In this talk, we propose an efficient numerical method to solve nonlinear filtering (NLF) problems. Specifically, we use the tensor train decomposition method to solve the forward Kolmogorov equation (FKE) arising from the NLF problem. Our method consists of offline and online stages. In the offline stage, we use the finite difference method to discretize the partial differential operators involved in the FKE and extract low-dimensional structures in the solution tensor using the tensor train decomposition method. In the online stage using the precomputed low-rank approximation tensors, we can quickly solve the FKE given new observation data. Therefore, we can solve the NLF problem in a real-time manner. Finally, we present numerical results to show the efficiency and accuracy of the proposed method.

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MS154

Stability-Preservation in Model Order Reduction of Stochastic Galerkin Systems

We consider linear dynamical systems, where parameters are replaced by random variables to perform an uncertainty quantification (UQ). The solution can be expanded in a series including orthogonal basis polynomials, which depend on the random variables. A truncation of the series generates a finite approximation. The stochastic Galerkin method yields a larger deterministic linear dynamical system for the unknown time-dependent coefficient functions. We investigate stability-preserving projection-based model order reduction (MOR) of the stochastic Galerkin systems. On the one hand, a transformation to a dissipative form of the system can be applied, where high-dimensional Lyapunov equations have to be solved. It follows that the reduced-order model is also dissipative and thus asymptotically stable, provided that a Galerkin-type MOR is used in contrast to a Petrov-Galerkin-type MOR. On the other hand, the stochastic Galerkin system is passive if it can be written in a port-Hamiltonian form. Again a Galerkin-type MOR preserves the passivity, which guarantees the Lyapunov stability of the reduced-order model. We present results of numerical computations using a test example.

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MS154

Energy-Stable Closure Modelling for Discretely Filtered Turbulent Flow

We propose a ROM-based closure model for turbulent flow

that conserves the total kinetic energy. For this purpose, we start by considering an energy-conserving DNS discretization which is too expensive to be used in multi-query applications. To reduce the computational cost, we introduce a discrete filter matrix. Applying this discrete filter to the DNS velocity vector, we get a discretely filtered velocity vector with significantly smaller dimension. The information that is lost in this filtering process we call subgrid velocity. When simulating the dynamics of the filtered velocity, we cannot neglect the effects of the subgrid velocity. To take these subgrid effects into account, we approximate the subgrid velocity within a reduced basis. The resulting model consists of the filtered velocity and the approximated subgrid velocity and has a significantly smaller dimension than the DNS model. In contrast to classical model order reduction, we do not aim at reproducing the complete dynamics of the DNS model but only the filtered velocity. By preserving the structure of the underlying DNS discretization, we guarantee the proposed reduced order model to be energy-conserving and hence Lyapunov-stable.

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MS154

Approximate Deconvolution Leray Reduced Order Model for Convection-Dominated Flows

Numerical stabilization techniques are frequently employed to mitigate the arising of spurious oscillations, a common occurrence in simulations of convection-dominated flows modeled by the incompressible Navier-Stokes equations, particularly when utilizing full order models (FOMs) in under-resolved or marginally-resolved scenarios. However, the precise role of numerical stabilization in the context of reduced order models (ROMs) for simulating convection-dominated, under- or marginally-resolved flows remains not well understood. Initially we present regularized reduced order models (Reg-ROMs) for the incompressible NS equations. In particular, we introduce a novel ROM based on approximate deconvolution [1], ADL-ROM, and compare it with L-ROM and G-ROM. In ADL-ROM, the aim is to deconvolve the filtered variable in L-ROM to increase its accuracy without compromising its stability. We think that this type of regularization can bring great benefits in different practical applications, especially in cardiovascular models. In the end, we show ADL-ROM numerical results, the comparison between the different ROMs and the analysis of the errors, alongside their implementation in RBniCSx. [1] A. Sanfilippo, I. Moore, F. Ballarin, T. Iliescu. Approximate deconvolution Leray reduced order model for convection-dominated flows. Finite Elements in Analysis and Design, volume 226, 2023.

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MS154

Evolve-Filter-Relax Regularization Strategies in Feedback Control for Convection-Dominated Navier-Stokes Equations at Full and Reduced Levels

In many scientific and industrial applications, the controllability of flows is an important task and the interest in such a topic is constantly growing. The main goal is to steer the flow regime towards a beneficial configuration (less turbulent, more laminar). In this setting, we propose a novel linear feedback control as a suboptimal (yet accurate) strategy to deal with the Navier-Stokes equations with large Reynolds, guaranteeing exponential convergence in time to the desired state. In numerical simulations, there might be a need for other stabilization strategies when the Reynolds number increases. We employ the Evolve-Filter-Relax (EFR) algorithm and we theoretically study the loss of convergence towards the beneficial state. Guided by the theoretical results, we propose an adaptive EFR (aEFR) approach that alleviates the numerical oscillations of the controlled setting, recovering the exponential convergence of the original problem. These theoretical results are tested numerically on a 2D flow past cylinder with Reynolds 1000 at the full and reduced order model level.

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MS155

Navigating Complexity in Causal Structure Learning Through Recursion

Recovering causal relationships within complex systems, particularly when latent variables and selection biases are in play, poses substantial computational and statistical challenges, often rendering the complete algorithms for this task impractical. While certain more practical approaches have been suggested, they often fall short in providing completeness guarantees. Our proposal introduces a sound and complete recursive constraint-based method designed to overcome these obstacles. Our approach, through a systematic process, identifies and eliminates specific variables during each iteration, streamlining the learning of causal MAGs. This recursive strategy results in a reduction of

both the number of conditional independence tests and the size of conditioning sets of each test, enhancing the algorithm's efficiency. We provide an upper bound on the number of required conditional independence tests for our approach, as well as a universal lower bound. The provided upper and lower bounds differ only by a factor equal to the number of variables in the worst case.

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MS155

On the Estimation of the Generalized Precision Matrix

For a collection of random variables with multivariate normal distribution the precision matrix completely encodes the conditional independence (CI) structure of the probabilistic graphical model. The generalized precision matrix (GPM), based upon second derivatives of the underlying density, has been proposed to uncover CI information for more general joint distributions. In this talk I discuss methods and issues of estimation of the GPM and its utility to assess CI of the underlying variables. Developments are complemented with illustrative examples.

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MS155

Towards Learning General Markov Networks

Markov networks graphically represent the conditional independence relationships between random variables, offering a visual aid to navigate uncertainties in probability theory with a wide application in fields including physics, chemistry, biology, and sociology. Existing work focuses on specific families of distributions and/or certain structures of graphs, and most of them can only handle variables of a single data type. In this talk, I will introduce a new characterization of conditional independence structure, named Generalized Precision Matrix (GPM). Inspired by previous research, GPM generalizes Markov network learning to handle general distributions for all data types (continuous, discrete, and mixed-type data) without assumptions on the functional relations among variables.

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MS156

Black-Box Uncertainty Quantification for Space Antenna Design

Many modern antenna systems, particularly for applications in telecommunication or earth observation, have significant mechanical complexity. This entails an often detailed design process, where the design is carefully revised to ensure the best performance. In particular, the electrical design often needs to take into account uncertainties in the mechanical design. A development project of a new software tool for uncertainty quantification of an antennas performance caused by the stochastic behaviour of design variables of the system has been performed in collaboration with ESA. The mathematical algorithms implemented in the tool allow for a general formulation, where uncertainty can be added to both geometrical and electrical parameters of the system. While such non-intrusive uncertainty quantification is not new in this community, the implementation details required are challenging. The users of the software tool have little knowledge of the algorithms involved, and only modest understanding of statistical quantities. The implementation, based on only black-box access to the simulation algorithms, has required numerous design choices both in terms of algorithms, modelling and presentation of output. The talk will briefly go over the software structure itself, and then highlight some of the necessary compromises required. Finally, we will look towards the future requirements for the software, imposed by the rapid progression of new antenna designs.

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MS156

A Rare Event Framework for Prediction of Dwell Fatigue in Aeroengine Components

The accurate prediction of dwell fatigue failure events in Titanium alloy engine rotating components operating under cold dwell service conditions is of critical importance in aerospace applications. These failure events are described by extreme value distributions necessitating the development and validation of physics-based, probabilistic cold dwell fatigue (CDF) life models that use advanced methods for rare event prediction. A framework is described that leverages transport maps to efficiently sample from complex probability distributions. These probability distributions serve as input to a physics-based model used to track the break up and rotation of microtextured regions (MTRs) during component forging. Our rare event framework ultimately will connect prediction tools to the optimization of processing paths in order to enable future life extension efforts.

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MS156

Data Assimilation and Inverse Problems for Oil Spill Response Operations

Oil spills represent one of the most impactful forms of anthropogenic pollution. Containment of such events is very cumbersome, in particular when the spill happens at sea. Forecasting models are combined with weather forecasts, aerial and satellite data to predict the possible trajectories of spills. Data assimilation techniques are used to update the state of the spill and refine forecasts. In many situations the source of the spill is not known, and authorities need to reconstruct the evolution of the spill to pinpoint potential responsibilities. In this talk we will present data assimilation and hindcasting techniques based on optimal and non-optimal transport, applied to use cases for oil spill response operations.

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MS156

Bilevel Optimization with a No-Reference Image Statistics Based Score-Preditor Loss

Variational models represents a classical tool, with an established theoretical background, to solve a variety of inverse problems in imaging. One of their drawback is the absence of guidelines to select their parameters. Bilevel optimization can exploit the basics idea of machine learning to train a task-dependent variational model through the use of a limited amount of data and computational cost. In this talk we discuss a strategy to develop an unsupervised loss function for one of these Bilevel optimization problems. Without using a ground truth, the loss function needs to be able to quantify directly how good an image is to a human eye. For this reason, we present and discuss a MSSIM predictor based on a differentiable version of the features of BRISQUE, a No-Reference image quality measure [Mittal, Moorty, Bovik. "No-Reference Image Quality Assessment in the Spatial Domain", 2012]. In order to reduce the uncertainty of the score predictor towards unseen images, we perform a data augmentation procedure to enrich the dataset that is used to train it. This model is tested on standard imaging problems, and although some of its elements are task-dependent, its framework is easily transposable to many other applications.

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MS157

Balancing-Based Model Reduction for Nonlinear Bayesian Inverse Problems

Solving Bayesian inverse problems quickly becomes computationally infeasible, especially when the underlying system is nonlinear and the dimension of the parameters to be inferred is large. We present an approach to model order reduction for such problems based on the system-theoretic concept of balanced truncation. We discuss the difficulties that arise in applying balanced truncation for Bayesian inference and nonlinear systems, and point out opportunities and limitations of balancing for nonlinear Bayesian inverse problems.

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MS157

A Multi-Fidelity Ensemble Kalman Filter with Adaptive Reduced Order Models

The use of model order reduction techniques in combination with ensemble-based methods for estimating the state of systems described by nonlinear partial differential equations has been of great interest in recent years in the data assimilation community. Methods such as the multi-fidelity ensemble Kalman filter (MFEnKF) and the multi-level ensemble Kalman filter (MLEnKF) have been developed and implemented in several papers and are recognized as state-of-the-art techniques. However, the construction of low-fidelity models in the offline stage, prior to solving the data assimilation problem, leads these methods into a trade-off between the accuracy and computational cost of the approximate models. In our work, we investigate the use of adaptive reduced-basis techniques in which the approximation space is modified (but not retrained) online based on the information extracted from the full-order solutions. This has the potential to simultaneously ensure good accuracy and low cost for the employed models and thus improve the performance of the multi-fidelity/multi-level methods.

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MS157

Emulating High-Dimensional Forward Models with Modified Kernel Flows

Remote sensing retrievals are typically formulated as Bayesian inverse problems. In this talk we consider inference of hyperspectral reflectance from imaging spectrometers such as SBG, EMIT, and AVIRIS-NG. These instruments make high-dimensional radiance measurements in the visible and shortwave infrared ranges, which are then used as data to solve Bayesian inverse problems. Due to the high volume of observations, methods such as Markov chain Monte Carlo are not usable in this context for operational use. In this talk we present a fast way to carry out hyperspectral reflectance retrievals by employing fast inversion algorithms and accurate Gaussian process-based radiative transfer emulation. In particular, we combine two recent developments: Accelerated Optimal Estimation and forward model emulation based on modified Kernel Flows (Gaussian process regression with a data-adapted kernel learned using a variant of cross-validation and increasingly sophisticated families of kernels). Together these developments have the potential to improve estimation accuracy while speeding up inference and dramatically reducing code complexity. The main emphasis will be on how the emulators are constructed. Time permitting, we will also briefly present how the emulation framework performs in a number of other problems.

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MS158

Detecting Causality in Dynamical Processes with the Information Imbalance of Distance Ranks

Uncovering causal relationships between time-dependent observables is a problem which goes at the heart of scientific research. However, this task is particularly challenging when data are collected without performing interventional experiments. Distinguishing a cause-effect relationship from a correlation is still considered an open problem, especially if the effect is triggered by the simultaneous variation of a large number of variables. As a major limitation, many available methods are often not able to distinguish the absence of causality from a weak causal link, bringing to false-positive discovery. Here, I will illustrate a method for causal detection based on the Information Imbalance of distance ranks, a statistical test capable of inferring the relative information content of different distance measures. Using both synthetic and real-world time series, I will show that our framework significantly mitigates the problem of false-positive detections, handling high-dimensional data that are challenging for other approaches.

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MS158

Statistical Parameter Identification of Pattern Formation Models

Pattern formation plays a key role during embryogenesis and the formation of multicellular structures. Since the seminal work of Alan Turing, these processes have been modelled by reaction-diffusion systems. In this theory, the destabilisation of spatially homogeneous equilibrium states leads to the formation of stable concentration structures, known as Turing patterns. Alternative hypotheses combine the dynamics of diffusing molecular signals with tissue mechanics or intracellular feedback. However, steady-state patterns strongly depend on initial conditions. As a result, the fixed parameters of the model always correspond to a family of patterns rather than a fixed solution. Additionally, in many experimental situations only limiting regimes are observable. Due to the severe limitation of information, measuring the difference between model output and pattern data becomes a challenging task and standard methods cannot be applied. For this situation, we develop a statistical approach that allows distinguishing the model parameters that correspond to given patterns. The method is first tested using different classes of pattern formation models and severely limited datasets. Next, the approach is used to fit the classical reaction-diffusion model of the chlorite-iodite-malonic acid (CIMA) reaction to the experimental pattern data.

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MS158

Likelihoods Instead of Likelihood-Free Inference for SDE Models

We present a variation of the Bayesian synthetic likelihood approach for the parameter estimation of stochastic differential equations. This technique allows for inference based on tailored but generic summary statistics based on data distributions. We also provide means to evaluate whether a given model fits the observational data only 'by chance', leading to a potentially 'good looking' posterior that could mislead a not-careful-enough user to rely on a biased model when trying to predict future outcomes of a system. As test cases, we will present the approach by employing models from the mathematical finance field, including comparison against other methods, such as maximum likelihood, filtering, and transition density estimation.

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MS158

Multilevel Monte Carlo Learning for High-Dimensional Feynman-Kac Representations of PDE Solutions

Solving high-dimensional PDEs is a fundamental challenge

in various fields, including mathematical finance. In this talk, we revisit an approach, initially pioneered by Beck et al., which leverages neural networks and the Feynman-Kac formula to construct numerical solution methods for linear PDEs. The essence of this approach lies in efficiently shifting the computational burden to an offline training process, thereby enabling near real-time computations during practical applications. However, in financial scenarios, such as pricing high-dimensional basket options, the need for frequent neural network retraining can still present a substantial obstacle. To address this challenge, we discuss different flavors of Multilevel Monte Carlo learning. This approach involves training several neural networks, each characterized by a specific approximation quality and computational complexity. Drawing inspiration from Giles' Multilevel Monte Carlo methodology, we significantly enhance the efficiency of the training process by shifting the bulk of the computational workload to training neural networks at coarse levels, where generating training data is cost-effective and which on the other hand allows us to minimize the number of training data sets required for fine-level neural network training. This is talk is based on joint work with Thomas Gerstner, Bastian Harrach, Theonille Mukamana, Lassi Roininen and Daniel Roth

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MS159

Dynamic Mode Decomposition Accelerates Uncertainty Quantification via Polynomial Chaos Expansion

Polynomial Chaos Expansion (PCE) is a model reduction technique that returns an approximation of the response provided by a high-fidelity model (HFM) in the random parameter space. PCE has shown to be a powerful tool to accelerate uncertainty quantification for a set of flow and transport problems. Training PCE is conveniently performed through a non-intrusive regression-based approach according to the Probabilistic Collocation Method. However, in the case of models with time-variant response, the computational cost of training PCE increases with the number of space-time locations where a number of HFM runs is required. Here, we investigate how this limitation is overcome by using Dynamic Mode Decomposition (DMD) which is a powerful factorization and dimensionality reduction technique for data sequences associated with complex dynamic systems. Specifically, we propose to use DMD to interpolate HFM data in time and inform PCE by substituting high-fidelity data with increasing replacement rates. We investigate the accuracy of the approach for uncertainty quantification related to flow and transport processes in heterogeneous porous media.

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MS159

Using Generative A.I. for Downscaling Ocean Models and Quantifying the Uncertainty

In ocean modeling, achieving high-resolution representation is critical for accurately capturing specific dynamics, such as submesoscale features in mesoscale-resolving ocean simulations. The current research employs generative AI, specifically score-based diffusion models, to address the inherent limitations of low-resolution models. By training on short-duration, high-resolution ocean simulations, the proposed method aims to bias correct low-resolution models, aligning them more closely with the statistics of high-resolution simulations. Notably, this approach is intrinsically tied to the statistics of the high-resolution data, promoting a more faithful replication of high-resolution dynamics. The overarching objective is to provide a computationally efficient technique to emulate high-resolution statistics and shed light on regional-scale information. This talk assesses the efficacy of AI-driven downscaling in replicating regional scale statistics of oceanic processes.

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MS159

Real-Time High-Resolution Co2 Geological Storage Prediction Using Nested Fourier Neural Operators

Carbon capture and storage (CCS) plays an essential role in global decarbonization. Scaling up CCS deployment requires accurate and high-resolution modeling of the storage reservoir pressure buildup and the gaseous plume migration. However, such modeling is very challenging at scale due to the high computational costs of existing numerical methods. This challenge leads to significant uncertainties in evaluating storage opportunities, which can delay the pace of large-scale CCS deployment. We introduce Nested Fourier Neural Operator (FNO), a machine-learning framework for high-resolution dynamic 3D CO2 storage modeling at a basin scale. Nested FNO produces forecasts at different refinement levels using a hierarchy of FNOs and speeds up flow prediction nearly 700,000 times compared to existing methods. By learning the solution operator for the family of governing partial differential equations, Nested FNO creates a general-purpose numerical simulator alternative for CO2 storage with diverse reservoir conditions, geological heterogeneity, and injection schemes. Our framework enables unprecedented real-time modeling and probabilistic simulations that can support the scale-up of global CCS deployment.

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MS160

UncertaintyQuantification.jl: Recent Developments and New Features

UncertaintyQuantification.jl is a new generalized open source framework for uncertainty quantification written in the Julia programming language. In this talk we present the latest features that have been implemented or are cur-

rently in development. Most importantly we introduce the work that has been undertaken to enable the propagation of imprecise probabilisties such as p-boxes. The system is designed to wrap around the existing algorithms and sampling schemes so that new propagation algorithms and different types of imprecise probabilities can be implemented with little code duplication. In addition, we present some benchmarks to highlight the performance of the framework.

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MS160

Chaospy: A Pythonic Approach to Polynomial Chaos Expansion

Polynomial chaos expansion is a popular method for extracting statistical metrics from solutions of forward problems with well characterized variability in the model parameters. Chaospy is a numerical implementation specifically developed to construct, manipulate and analyze polynomial chaos expansions using the high modularity and expressiveness of Python. The toolbox allows for implementation of an expansion using only a handful lines of code. Chaospy is a development foundry that allows for easy experimentation with custom features beyond the scope of standard implementation. To demonstrate the capabilities of the Chaospy toolbox, this talk will demonstrate how polynomial chaos expansions can be applied on an stochastically dependent random variable. This includes constructing dependent random variables, and constructing the uncertainty quantification using a couple of approaches.

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MS160

UQ[py]Lab 1.0 - From Matlab to Python, Through the Cloud

Uncertainty quantification (UQ) is growing in all fields of applied sciences, including civil and mechanical engineering, applied mathematics, physics, economics, industry, etc.. Such a wide range of usage scenarios brings a significant challenge to the task of UQ software design and development, as the associated computational workflows are likely to be just as diverse, with different programming languages and operating systems in each community. The widespread success of UQLab has been in large part due to its intuitive design, ease of use and extended documentation, but its reliance on the Matlab programming language has somewhat limited its adoption in several communities, especially those more python-centric. To work around this complex problem, while keeping a single development pipeline across different programming languages, we started the UQCloud project in 2020, aiming at providing a language-independent, cloud-based port of UQLab. UQCloud allows us to seamlessly integrate the latest version of UQLab into a software-as-a-service wrapper, with a secure web API easily accessible from any programming language. After several years of development and an extensive beta testing phase, we are happy to announce the first production release of UQ[py]Lab, the python client for UQCloud. In this contribution, we will present the current state of the project, including several of the challenges that it posed, and an outlook to its development perspectives.

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MS160

UQpy: An Open-Source Python Toolbox and Development Environment for Uncertainty Quantification

UQpy is an open-source python toolbox that facilitates a wide-range of UQ tasks in physical, engineering, and mathematical systems. UQpy is a highly modularized, object-oriented package that is designed for both flexible use and for the natural extension to include new methods. Each module of UQpy is dedicated to a specific set of UQ tasks; currently comprised of 11 modules for tasks as diverse as, inference, reliability, and surrogate modeling. Its modularity also allows its various pieces to be assembled into a larger workflows to support efforts that require several UQ tools. UQpy is conveniently written in Python, which serves as a natural language for wide-ranging scientific computing applications. Moreover, UQpy serves as an ideal platform to test and implement new UQ techniques. The latest release, v4.1, introduces an improved code architecture, resulting in a more straightforward and user-friendly experience for both users and developers. To ensure the reliability and quality of the software, UQpy employs Continuous Integration, which adheres to rigorous code quality standards, and automated testing to validate the scientific results it produces. Additionally, UQpy is packaged and distributed in a system-agnostic format, making it accessible through various packaging archives such as PyPi, conda-forge, and Docker images. This approach broadens the reach of UQpy and overcomes system-specific limitations, making it a valuable resource for the scientific community.

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MS161

Affine Invariant Ensemble Transform Methods to Improve Predictive Uncertainty in Neural Net-

works

The problem of sampling from a target distribution is fundamental to Bayesian statistics, machine learning, and data assimilation.Since its introduction, the ensemble Kalman filter (EnKF) has been a popular choice for performing data assimilation tasks due to its robustness and wide applicability.In this talk, we consider the problem of performing Bayesian inference for logistic regression using appropriate extensions of the EnKF. We propose two interacting particle systems that sample from an approximate posterior and prove quantitative convergence rates of these interacting particle systems to their mean-field limit as the number of particles tends to infinity. Furthermore, we apply these techniques, examine their effectiveness as methods of Bayesian approximation for quantifying predictive uncertainty in ReLU networks,and compare them to the state-of-the-art.

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MS161

Non-Gaussian Extensions of the Ensemble Kalman Filter: Gaussian Anamorphosis and Two-Step Ensemble Filters

EnKFs make a Gaussian approximation of the joint distribution of the state and observations. Gaussian anamorphosis methods relax this assumption to that of a Gaussian copula between the state and observations, while methods like the ensemble conjugate transform filter relax this assumption even further. Two-step ensemble filters grow out of a two-step implementation of the EnKF devised by Anderson ("A local least-squares framework for ensemble filtering," 2003). Because two-step ensemble filters are not based on transforming to a Gaussian distribution, they generalize to non-Gaussian distributions differently than anamorphosis and related methods. This talk presents EnKFs, Gaussian-anamorphosis EnKFs, and two-step ensemble filters from a unified perspective. It then presents examples of their performance in the Lorenz-96 model, and in the context of assimilating discrete observations of wind direction for historical reanalysis.

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MS161

Discretization and Ensemble Approximation Error for Ensemble Kalman Updates in Function Spaces

Many inverse problems and data assimilation tasks are most naturally formulated in a function space setting. To handle these problems numerically, the function space must be discretized. We review a computational framework for discretizing inverse problems in an infinite-dimensional Hilbert space and formulate the ensemble Kalman update in this framework. In the linear-Gaussian setting, we characterize the discretization error and the expected ensemble approximation error for the ensemble Kalman update at a finite ensemble size. The approximation error is controlled a notion of effective dimension related to the spectral decay of the prior covariance operator. We show that the effective dimension of the discretized problem is controlled by the effective dimension of the continuum problem, which is finite. As such, the estimation error remains controlled as the discretization is refined despite the nominal dimension of the problem growing arbitrarily large.

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MS162

Graph-based Surrogates for CFD Simulations in Parametrized Domains

In the context of inverse engineering, optimal design, and uncertainty quantification, mesh-based computational fluid dynamics (CFD) simulations for industrial applications can be prohibitively expensive. Furthermore, in industrial settings, it is often the case that computational domains must adapt to continuously changing environmental and operational scenarios. In this work, we develop neural network surrogates to accelerate CFD simulations characterized by parametrized, three-dimensional computational domains; our ensemble of architectures is based on MeshGraphNets and it is specifically designed for fluid simulations with varying input parameters, including parametrized input geometries. In this context, we explore an attention mechanism based on physics as a means to mix learned communication with physical constraints; we term this approach physics-informed attention. We test and compare the accuracy of the proposed surrogates on three-dimensional parametrized channel flow simulations. Comparisons with other baseline methods are also presented.

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MS162

Space-Time Shape Uncertainty for the Inverse Problem of Electrocardiography

In electrocardiography, the "classic" inverse problem is the reconstruction of electric potentials at a surface enclosing the heart from remote recordings at the body surface and an accurate description of the anatomy. The latter being affected by noise and obtained with limited resolution due to clinical constraints, a possibly large uncertainty may be

perpetuated in the inverse reconstruction. This talk concerns the study of the effect of shape uncertainty on the forward and the inverse problem of electrocardiography. To this aim, the problem is first recast into a boundary integral formulation and then discretized with a collocation method to achieve high convergence rates and a fast time to solution. The shape uncertainty of the domain is represented by a random deformation field defined on a reference configuration. We propose a periodic-in-time covariance kernel for the random field and approximate the KarhunenLove expansion using low-rank techniques for fast sampling. The spacetime uncertainty in the expected potential and its variance is evaluated with an anisotropic sparse quadrature approach and validated by a quasi-Monte Carlo method. We present several numerical experiments on a simplified but physiologically grounded two-dimensional geometry to illustrate the validity of the approach.

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MS162

Non-Intrusive Mesh-Free Surrogate Models in Variable Shape Domains

In this presentation, we present a novel surrogate model, based on artificial neural networks (ANNs), which applies to differential problems whose solution depends on physical and geometrical parameters. We employ a mesh-less architecture, thus overcoming the limitations associated with image segmentation and mesh generation required by traditional discretization methods. Our method encodes geometrical variability through scalar landmarks, such as coordinates of points of interest. We present proof-of-concept results obtained with a data-driven loss function based on simulation data. Nonetheless, our framework is non-intrusive and modular, as we can modify the loss by considering additional constraints, thus leveraging available physical knowledge. Our approach also accommodates a universal coordinate system, which supports the surrogate model in learning the correspondence between points belonging to different geometries, boosting prediction accuracy on unobserved geometries. Finally, we present two numerical test cases in computational fluid dynamics involving variable Reynolds numbers as well as computational domains of variable shape. The results show that our method allows for inexpensive but accurate approximations of velocity and pressure, avoiding computationally expensive image segmentation, mesh generation, or re-training for every new instance of physical parameters and shape of the domain.

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tion Using Deep Reinforcement Learning

Model-informed precision dosing (MIPD) leverages prior knowledge and biomarker data for individualized drug dosing. Such dose adjustments are particularly important in fields like oncology, with narrow therapeutic windows and severe dose-limiting effects such as neutropenia. MIPD approaches have been proposed in this field but estimating model parameters can be a crucial factor in describing the personalized trajectories of individual patients. Furthermore, it might be necessary to choose control parameters that can be understood as decisions/actions performed related to the specific therapeutic treatment of a patient. Advanced machine learning techniques in the form of reinforcement learning (RL) have been successfully applied to overcome the computational challenges of deriving optimal treatment plans personalized to individual patients. This research introduces an innovative paradigm that leverages neural networks to amplify the effectiveness and reach of Monte Carlo sampling in Reinforcement Learning. By combining the strengths of neural networks with Monte Carlo methods, our approach significantly improves value function estimation, accelerates learning, and extends the applicability of Monte Carlo techniques to a broader array of RL scenarios, thereby advancing the field of autonomous decision-making systems.

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MS163

On Backward Smoothing Algorithms

(joint work with Hai-Dang Dau, Oxford University) In the context of state-space models, skeleton-based smoothing algorithms rely on a backward sampling step which by default has a $O(N^2)$ complexity (where N is the number of particles). Existing improvements in the literature are unsatisfactory: a popular rejection sampling – based approach, as we shall show, might lead to badly behaved execution time; another rejection sampler with stopping lacks complexity analysis; yet another MCMC-inspired algorithm comes with no stability guarantee. We provide several results that close these gaps. In particular, we prove a novel non-asymptotic stability theorem, thus enabling smoothing with truly linear complexity and adequate theoretical justification. We propose a general framework which unites most skeleton-based smoothing algorithms in the literature and allows to simultaneously prove their convergence and stability, both in online and offline contexts. Furthermore, we derive, as a special case of that framework, a new coupling-based smoothing algorithm applicable to models with intractable transition densities. We elaborate practical recommendations and confirm those with numerical experiments.

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MS163

filtering problems where the state space can have millions of degrees of freedom. I will also present some application of particle filters for solving geo-physical fluid dynamics data assimilation problems.

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MS163

A Divide and Conquer Sequential Monte Carlo Approach to High Dimensional Filtering

We propose a divide-and-conquer approach to filtering which decomposes the state variable into low-dimensional components to which standard particle filtering tools can be successfully applied and recursively merges them to recover the full filtering distribution. It is less dependent upon factorization of transition densities and observation likelihoods than competing approaches and can be applied to a broader class of models. Performance is compared with state-of-the-art methods on a benchmark problem and it is demonstrated that the proposed method is broadly comparable in settings in which those methods are applicable, and that it can be applied in settings in which they cannot. Joint work with Adam M Johansen.

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MS164

Data Driven Modeling of Stochastic Systems

We present a numerical framework for learning unknown stochastic dynamical systems using measurement data. Termed stochastic flow map learning (sFML), the new framework is an extension of flow map learning (FML) that was developed for learning deterministic dynamical systems. For learning stochastic systems, we define a stochastic flow map that is a superposition of two sub-flow maps: a deterministic sub-map and a stochastic sub-map. The stochastic training data are used to construct the deterministic sub-map first, followed by the stochastic sub-map. The deterministic sub-map takes the form of residual network (ResNet), similar to the work of FML for deterministic systems. For the stochastic sub-map, we employ a generative model, particularly generative adversarial networks (GANs) in this paper. The final constructed stochastic flow map then defines a stochastic evolution model that is a weak approximation, in term of distribution, of the unknown stochastic system. A comprehensive set of numerical examples are presented to demonstrate the flexibility and effectiveness of the proposed sFML method for various types of stochastic systems.

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MS164

Bayesian Model Selection for Capturing Closure Models in Nonlinear Dynamics

Constitutive models play a crucial role in the analysis of dynamical systems in numerous engineering and scientific disciplines. These models provide a systematic and quantitative framework for (a) understanding the behavior, and (b) predicting the evolution of complex systems. Oftentimes such models, by design, overlook certain aspects of the underlying physics for a variety of reasons, such as the need to reduce computational requirements to simulate those systems or the lack of complete understanding of complex physical phenomenon. As models continue to be used in exploring new regimes of operation, previously overlooked and unresolved dynamics start to gain significance due to declining predictive accuracies. In order to maintain a target level of predictive accuracy in such settings, it is important to capture closure terms using data-driven approaches. We promote the use of stochastic dynamical models to capture information on missing closure terms, to be trained within a data assimilation setting. This talk will examine the utility in applying advanced Bayesian model selection techniques to answer questions related to the type of stochastic model needed to capture such information. For numerical investigation, we consider a slight modification of the nonlinear Duffing oscillator to examine the efficacy of the proposed framework.

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MS164

Multi-Time Inversion for the Calibration of Expensive Chaotic Models

Computer models traditionally used for weather and climate prediction have extremely high computational costs, which impedes their use in education, scientific exploration, and uncertainty quantification. Physics-based reduced models exist but their utility is limited, in part, because their calibration poses a host of difficulties, including chaotic dynamics that prevent the use of adjoint methods, computational costs that become unreasonable when sampling approaches require many forward runs with long ergodic trajectories, and large existing code bases that require black box approaches. Recently, Kalman inversion methods have shown promise by providing approximate derivatives of parameters in black box models in order to reach convergence using relatively few forward model runs. Building on those methods, and inspired by work in consistency testing for climate models, we demonstrate that using samples of ultra-short trajectories can result in significant reduction of the calibration cost on both classical chaotic test cases and a reduced global circulation model. In contrast to other multi-fidelity methods, our ability to use the same model resolution throughout calibration avoids issues with resolution-dependent parameters common in climate and weather models.

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MS165

Smoothing Gradient Descent with Probability Distributions

This talk will focus on smoothing both gradient descent and stochastic gradient descent by convolving the target function with a probability distribution (e.g., compactly

supported or normal distributions). Theoretical results for convergence rates will be provided for L-smooth objective functions and improved upon in the Gaussian setting. Numerical examples illustrating the theoretical results as well as advantages and disadvantages of certain distributions will be discussed.

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MS165

High-Dimensional Optimization with a Novel Nonlocal Gradient

We develop a nonlocal gradient that skips small local minima and captures major structures of the loss's landscape in optimization of high-dimensional, multimodal functions. The key idea is applying Gaussian smoothing directionally and conduct 1D long-range exploration with large smoothing radius along each orthogonal direction. Gauss-Hermite quadrature rule is employed to obtain an accurate estimator of the nonlocal gradient. We provide convergence theory and demonstrate the performance of our method in several high-dimensional benchmark tests.

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MS165

Implicit Methods for Deep Learning on Graphs

In this talk, I will present two implicitly defined graph neural networks (GNNs) based on finding the fixed point of equilibrium equation and parameterizing diffusion PDE on graphs. These new implicit GNNs can effectively overcome the over-smoothing issue of GNNs and learn with minimal supervision. Also, these new models enjoy computational and memory efficiency when applying operator splitting schemes and the adjoint method for their training and inference.

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MS165

Stochastic Average Model Methods

We consider finite-sum minimization problems in which the summand functions are computationally expensive, making it undesirable to evaluate all summands on every iteration. We present the idea of stochastic average model methods trust-region solver POUNDERS.

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MS166

Learning Functionals for Wasserstein Gradient Flows on SE(2)

We consider the problem of solving inverse problems, and doing image processing tasks by lifting the problems from R^2 to SE(2) and using Wasserstein gradient flows on the Lie group SE(2). We show that there is merit in working with the gradient flow in the higher dimensional setting of this Lie group, and wish to automatically learn the functional over which to do the gradient flow in a supervised manner.

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MS166

Optimal Sampling for Least Squares and Interpolation in General Spaces

We address the problem of function approximation in a finite dimensional space using standard weighted least squares. It is well established that least squares offer greater stability than interpolation but this comes at the cost of requiring a larger sampling budget. We demonstrate that it is possible to achieve near-optimal approximation error, in an expected L^2 sense, when the sample size m exceeds the dimension n of the approximation space by a constant ratio. This represents an improvement over similar recent findings, which necessitate a large ratio and are based on random sampling techniques involving renormalized Christoffel functions, as in the work of Cohen/Migliorati. Additionally, we provide novel results related to optimal sampling techniques for interpolation. We reveal an unconventional strategy for constructing interpolation nodes with relatively moderate Lebesgue constants. We were able to derive our results by shifting from independent and identically distributed (i.i.d.) sampling to greedy dependent sampling. The proposed sampling algorithms use ideas from graph sparsification, inspired by the papers of Batson/Spielman/Srivasta and Lee/Sun.

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MS166

classification problems, we often encounter discontinuous functions. Approximating these, especially in high dimensions, is a serious challenge and essentially impossible using classical tools. We will show that, in the relam of machine learning with deep neural networks, these issues can often be overcome and optimal approximation rates (often without curse of dimensionality) can be achieved.

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MS166

Transformers and Function Approximation: What Can We Learn About the Attention Scheme?

The introduction of transformers led to an impressive performance jump in natural language processing. The most prominent example is Chat-GPT, which is now widely used and makes AI systems available to a large audience. In addition, Transformer show also for other applications impressive results, like computer vision and biology. The main building block of Transformers is the attention scheme. The attention mechanism allows us to connect every element in a sequence with every other element. Therefore, it is substantially different from feedforward networks. Besides the great success of Transformers, there is still little known from the theoretical perspective and there are many open questions. One big question is: Why are Transformers so powerful? We want to approach this question from the perspective of function approximation. We investigate in experiments how the approximation differs from classical approximation schemes and deep feedforward networks and combine these findings with the theoretical analysis of expressive power.

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MS167

A Heteroencoder Architecture for Prediction of Failure Locations in Porous Metals Using Variational Inference

In this work we employ an encoder-decoder convolutional neural network to predict the failure locations of porous metal tension specimens based only on their initial porosities. The process we model is complex, with a progression from initial void nucleation, to saturation, and ultimately failure. The objective of predicting failure locations presents an extreme case of class imbalance since most of the material in the specimens does not fail. In response to this challenge, we develop and demonstrate the effectiveness of data- and loss-based regularization methods. Since there is considerable sensitivity of the failure location to the particular configuration of voids, we also use variational inference to provide uncertainties for the neural network predictions. We connect the deterministic and Bayesian convolutional neural network formulations to explain how variational inference regularizes the training and predictions. We demonstrate that the resulting predicted variances are effective in ranking the locations that are most likely to fail in any given specimen.

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MS167

Neural Operators for Stochastic Modeling of System Response to Natural Hazards

Traditionally, deep neural networks (DNNs) have been employed to learn the mapping between finite dimensional Euclidean spaces. However, recent research has focused on using DNNs to learn operators mapping infinite-dimensional function spaces. In this work, we employ two state-of-the-art neural operators, deep operator network (DeepONet) and the Fourier neural operator (FNO) for performance-based evaluation of structural systems exposed to natural hazards. The DeepONet provides a flexible paradigm that does not limit the architecture of the constituent networks, termed branch and trunk networks. Specifically, we propose a Fast Fourier Transform based DeepONet (FFT-DeepONet), which inputs the Fourier modes in the trunk network through a fully connected feed forward neural network. FNO parameterizes the integral kernel in the Fourier space, and can be conceptualized as a DeepONet with a particular branch network architecture and trunk net expressed by discrete trigonometric basis functions. To demonstrate the efficiency and applicability of the frameworks to natural hazards, two problems are considered. First, we employ the operators to predict the response of a building to extreme stochastic winds. In the second, we forecast the seismic response of a six-story shear building subjected to various ground motion records. The trained surrogate models achieve high accuracy while being orders of magnitude faster than the original high-fidelity models.

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MS167

Methods and Performance of Uncertainty Quantification of Neural Network Models of Time-Evolving Processes

Time-evolving processes, such as local weather, stock pricing, reaction-diffusion systems and materials undergoing

deformation, represent a large and important class of modeling challenges. A variety of neural network (NN) models have arisen to meet this challenge, including well-known *recurrent neural networks* such as LSTM [Hochreiter,1997]

and GRUs [Cho,2014]. By incorporating hidden states and gating mechanisms, these networks vary in how they forecast and how the incorporate history. Others such as neural ODEs (NODEs) [Chen,2018;Dupont,2019] and causal convolutional NNs [Chen,2020] resemble more traditional models of time evolving systems. A variety of methods for uncertainty quantification for these representations beyond standard methods, such as stochastic NODEs [Xu,2022] and Bayesian NNs [Dandekar,2020], have followed the development of the deterministic models. This talk with be an exploration how uncertainty propagates within these NN frameworks, and how principles such as causality constrain the output. The exploration will use exemplars from chemistry and material physics.

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MS168

Estimation of Small Quantile Sets Using a Sequential Bayesian Strategy

Given a numerical simulator of a physical phenomenon or system, one often seeks to determine the set of inputs that lead to values with specified properties. This type of problem, broadly known as "set inversion," has several variants, depending on the properties sought for the outputs. In this communication, we concentrate on a specific robust set inversion problem termed "quantile set inversion" (QSI). In this context, the function of interest has both deterministic and uncertain inputs. The objective within this framework is to estimate the set of deterministic inputs so that the probabilitywith respect to the distribution of the uncertain inputsof the output variables falling within a given range is below a given threshold. To address this problem, we recently proposed (Ait Abdelmalek-Lomenech, Bect, Chabridon & Vazquez, arXiv:2211.01008v2, 2023) a sequential Bayesian sampling strategy based on the Stepwise Uncertainty Reduction (SUR) principle. We now suggest an adaptation of this method, employing sequential Monte Carlo (SMC) sampling, to tackle cases where the set to be estimated is small compared to the full domain of deterministic inputs.

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MS168

Multifidelity Risk Assessment for Nonlinear Systems under High-Dimensional Dependent Random Variables

Risk assessment is a key step in risk-averse design and uncertainty quantification of critical infrastructure and engineering systems. Computing risk measures, by their nature of being tail integrals, however, is computationally expensive. This is further exacerbated when the system models are expensive to simulate. We present multifidelity methods for the case of Conditional Value-at-Risk (CVaR) estimation for nonlinear systems under high-dimensional dependent random inputs. These methods are built on the basis of dimensionally decomposed generalized polynomial chaos expansion (and Kriging) which allow us to accurately approximate nonlinear and nonsmooth random outputs. The surrogate models are then used to compute the risk measures via (1) Monte Carlo simulation (MCS) and (2) multifidelity importance sampling (MFIS). We present illustrative academic results and demonstrate the scalability of the proposed methods and their applicability to complex engineering problems are demonstrated on a two-dimensional composite laminate with 28 (partly dependent) random inputs and a three-dimensional composite T-joint with 20 (partly dependent) random inputs.

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MS168

Insight from the Kullback-Leibler Divergence into Adaptive Importance Sampling Schemes for Rare Event Analysis in High Dimension

We study two adaptive importance sampling schemes for estimating the probability of a rare event in the high-dimensional regime $d \to \infty$ with d the dimension. The first scheme, motivated by recent results, seeks to use as auxiliary distribution a projection of the optimal auxiliary distribution (optimal among Gaussian distributions, and in the sense of the Kullback–Leibler divergence); the second scheme is the prominent cross-entropy method. In these schemes, two samples are used: the first one to learn the auxiliary distribution and the second one, drawn according to the learnt distribution, to perform the final probability estimation. Contrary to the common belief that the sample size needs to grow exponentially in the dimension to make the estimator consistent and avoid the weight degeneracy

phenomenon, we find that a polynomial sample size in the first learning step is enough. We prove this result assuming that the sought probability is bounded away from 0. For the first scheme, we show that the sample size only needs to grow like rd with r the effective dimension of the projection, while for cross-entropy, the polynomial growth rate remains implicit although insight on its value is provided. In addition to proving consistency, we also prove that in the regimes studied, the importance sampling weights do not degenerate.

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MS168

Consensus-Based Rare Event Estimation

We introduce a new algorithm for rare event estimation based on adaptive importance sampling. We consider a smoothed version of the optimal importance sampling density, which is approximated by an ensemble of interacting particles. The particle dynamics is governed by a McKean-Vlasov stochastic differential equation, which was introduced and analyzed in [Carrillo et al., Stud. Appl. Math. 148:1069-1140, 2022] for consensus-based sampling and optimization of posterior distributions arising in the context of Bayesian inverse problems. We develop automatic updates for the internal parameters of our algorithm. This includes a novel time step size controller for the exponential Euler method, which discretizes the particle dynamics. The behavior of all parameter updates depends on easy to interpret accuracy criteria specified by the user. We show in numerical experiments that our method is competitive to state-of-the-art adaptive importance sampling algorithms for rare event estimation, namely a sequential importance sampling method and the ensemble Kalman filter for rare event estimation.

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MS169

Efficient Expected Information Gain Estimators under Nuisance Uncertainty in the Context of Digital Twins

Optimal experimental design (OED) requires repeated evaluation of the expected information gain (EIG) functional. This entails solving a nested integration problem where the inner integral is separated from the outer integral by the logarithm. For many practical applications, both integrals must be estimated numerically, thus necessitating efficient estimators. Uncertainty regarding the parameters of interest is often accompanied by additional nuisance uncertainty. Quantifying this latter uncertainty introduces a second inner integral. Whether parameters are of interest or constitute a nuisance is ultimately guided by the intentions of the experimenter. We propose two novel estimators for the EIG under nuisance uncertainty utilizing the Laplace approximation, which has been successfully applied in OED problems to make computations more affordable. A digital twin models a physical system by repeatedly observing and subsequently making predictions about its physical counterpart, whichcan then be used to control the physical system.Finding the OED of a digital twin, i.e., placing sensors such that observational data is collected efficiently, is a process guided by the optimal control problem. Which parameters require focusing on may depend on the current state of the physical system.Estimating the EIG under nuisance uncertainty provides a comprehensive way to adjust to different objectives in the experimental design while rigorously quantifying uncertainties.

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MS169

Optimization Based Methods for Sample Selection in Semi-Supervised Learning

We present results on experimental design for pool-based active learning for multiclass classification using multinomial logistic regression. Given a trained classifier we seek to select a small number of new points for labeling. Once the points have been manually labeled, we add them to the training set and we retrain the classifier. The problem is to select points that improve the classification accuracy as much as possible. Here we present a theoretical analysis using the Fisher information ratio that establishes lower

and upper bounds for the generalization error and propose a regret minimization algorithm to select the samples. We compare our algorithms with state of the art and show that our algorithm consistently produces the smallest classification error in the multiclass logistic regression setting, as demonstrated through experiments on MNIST, CIFAR-10, and 50-class ImageNet.

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MS169

Optimal Experimental Design of Flightpath Planning Using a Digital Twin

Digital twins (DT) represent computational models of physical systems that continuously assimilate observational data to model and predict the behaviors of its physical twin. We propose an optimization model that selects observation trajectories for maximizing information gain and reducing uncertainty in a DT. The optimization problem corresponds using an optimal-experimental-design (OED) problem to provide the objective value for the control of an observational trajectory. We demonstrate our approach using a reaction-advection-diffusion equation that models the spread of pollutants in a system, implemented in Fenics. We examine the impact of different objective functions of the OED problem and different flightpath forms on our formulation.

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MS169

Rare Event Estimation in Complex Physics Models

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MS171

Deep GP Priors for Bayesian Inverse Problems

Recent theoretical advances justify the use of deep Gaussian process priors for Bayesian nonlinear regression and density estimation where the true function of interest has convolutional structure. Similar advances have shown that (single) Gaussian process priors perform well for Bayesian inverse problems. We combine these two lines of research, showing that deep GP priors can be more effective for inverse problems than single GP priors in the presence of compositional structure. However, we also highlight a key limitation with this approach: that Sobolev structure of PDE-based inverse problems, which can be leveraged when using GP priors, does not play nicely with compositional structure, so that it seems unlikely a deep GP approach can achieve a (frequentist) minimax rate in this setting.

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MS171

Posterior Contraction for Deep Gaussian Process Priors

We study posterior contraction rates for a class of deep Gaussian process priors applied to the nonparametric regression problem under a general composition assumption on the regression function. It is shown that the contraction rates can achieve the minimax convergence rate (up to log n factors), while being adaptive to the underlying structure and smoothness of the target function. The proposed framework extends the Bayesian nonparametric theory for Gaussian process priors. We discuss the relationship with deep neural networks and the many numerical challenges.

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MS171

Convergence Rates of Non-Stationary and Deep Gaussian Process Regression

Gaussian processes have proved to be a powerful and flexible tool in the reconstruction of functions given a set of known training points, with applications in machine learning, optimisation and data assimilation. However, they can be limited when the functions being reconstructed are of a non-stationary or anisotropic nature. Deep Gaussian processes, constructed using a hierarchical process where the inputs to a Gaussian process are themselves Gaussian processes, aim to give a more flexible approach to function reconstruction. We look at convergence rates of these deep Gaussian processes in terms of the number of known training points. We also show that deep Gaussian process regression achieves considerably better results than standard Gaussian process regression when reconstructing non-stationary and anisotropic functions.

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MS171

Spatiotemporal Gaussian Processes Defined by a New Class of Fractional Parabolic Spdes

A new class of space-time fractional parabolic stochastic evolution equations driven by Gaussian white noise is introduced, and its suitability for spatiotemporal statistical modelling is investigated. As a first step, mild and weak solution concepts are defined for which existence, uniqueness and equivalence results are established. Then, spatial regularity and mean-square temporal smoothness of the mild solution processes are quantified. These findings show that the smoothness in time and space as well as the degree of separability are governed by three model parameters, which can be fit to data during statistical inference. Moreover, characterizing the (long-time) covariance structure of this model class shows that it meaningfully generalizes the widely used (spatial) Matrn and WhittleMatrn models to spacetime.

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MS172

A Bi-Fidelity Strategy for Optimization under Uncertainty for Robust Trajectory Generation

We test a simple bi-fidelity strategy for accelerating trajectory optimization under uncertainty in the presence of robust constraints. Our approach combines the accuracy of high-fidelity models with the computational efficiency of low-fidelity counterparts to increase the accuracy of constraint computation for a given cost. Specifically, we accelerate sample average approaches that use high-fidelity models, with additional samples of low-fidelity models for assessing whether or not a risk constraint is violated. The low-fidelity model's purpose is thus to reduce the uncertainty in the estimate of constraint violation, at the expense of introduction of bias. Our empirical test on a simulation of glider dynamics tasked with avoiding a region indicates an order-of-magnitude less failures using the bi-fidelity strategy.

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MS172

Residual-based Error Corrector Operator to Enhance Accuracy and Reliability of Neural Operator Surrogates of Nonlinear Variational Boundary-value Problems

This work focuses on developing methods for approximating the solution operators of a class of parametric partial differential equations via neural operators. Neural operators have several challenges, including the issue of generating appropriate training data, cost-accuracy trade-offs, and nontrivial hyperparameter tuning. The unpredictability of the accuracy of neural operators impacts their applications in downstream problems of inference, optimization, and control. A framework based on the linear variational problem that gives the correction to the prediction furnished by neural operators is considered based on earlier work in JCP 486 (2023) 112104. The operator, called Residual-based Error Corrector Operator or simply Corrector Operator, associated with the corrector problem is analyzed further. Numerical results involving a nonlinear reactiondiffusion model in two dimensions with PCANet-type neural operators show almost two orders of increase in the accuracy of approximations when neural operators are corrected using the correction scheme. Further, topology optimization involving a nonlinear reactiondiffusion model is considered to highlight the limitations of neural operators and the efficacy of the correction scheme. Optimizers with neural operator surrogates are seen to make significant errors (as high as 80 percent). However, the errors are much lower (below 7 percent) when neural operators are corrected.

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MS172

Reducing Uncertainty for Complex Systems Through Multifidelity

Operator learning for complex nonlinear systems is increasingly common in modeling multi-physics and multi-scale systems. However, training such high-dimensional operators requires a large amount of expensive, high-fidelity data, either from experiments or simulations. In many cases, we may not have access to sufficient high-fidelity data to train, however we may have a large amount of low-fidelity data that is less accurate with greater uncertainty associated with it. The question is how to combine the low-fidelity and high-fidelity data to create a model that is capable of training more accurately than using the low- or high-fidelity data alone. In this work, we present a composite Deep Operator Network (DeepONet) for learning using two datasets with different levels of fidelity to accurately learn complex operators when sufficient high-fidelity data is not available. We show that the addition of a small amount of high-fidelity data, or physics-informed training, can overcome uncertainty due to highly noisy low-fidelity data, reducing the error in the final prediction.

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MS173

A Retraction Perspective on Dynamical Low-Rank Approximation

Retractions play a crucial role in algorithms designed to tackle optimization problems on smooth manifolds, ensuring that the iterates consistently remain within the man-

ifold. In this contribution, we investigate the use of retractions in the numerical integration of differential equations on fixed-rank matrix manifolds, a domain closely associated with Dynamical Low-Rank (DLR) approximation techniques. We demonstrate how retractions can be employed to explore well-known DLR techniques, such as the KSL and KLS algorithms, and to devise novel approaches. In particular, we demonstrate that these retractions are well-suited for constructing curve approximations on manifolds, with a local truncation error of order three. This showcases new perspectives on addressing current time-accuracy constraints in recent robust DLR algorithms. As a result, we introduce two innovative numerical integration schemes applicable to differential equations on general manifolds: the accelerated forward Euler (AFE) method and the Ralston-Hermite (RH) method. The latter extends the use of retractions beyond optimization, covering other computational tasks on manifolds, such as interpolation.

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MS173

Low-rank Dynamical Algorithms for State Estimation of Hamiltonian Systems

This talk focuses on the inverse problem of reconstructing an unknown function u from a finite set of measurements, under the assumption that u is the output of a parametric differential equation with unknown input parameters. Typically, the target function u belongs to an infinite-dimensional Hilbert space and the geometry of the solution set $\mathcal{M}$ is not known *a priori*. One way to reduce the complexity of the problem is to approximate $\mathcal{M}$ by a linear, finite dimensional subspace V using model order reduction, and to search for an approximation $u^* \in V$ to the state u. It is however known that such approach become ineffective for approximating the dynamics of transport problems. In this talk we will discuss how to address inverse problems for wave phenomena in the framework of Hamiltonian systems. The method combines symplectic dynamical low-rank approximation to update V with dynamical placement of the sensors to ensure an accurate reconstruction at all times.

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MS173

A Nonlinear Reduced Basis Approximation of Discrete Contact Problems in Crowd Motion

In this work we develop new model reduction approaches to predict the solutions of time-dependent parametrized problems describing crowd motion in the presence of obstacles. The problem of interest is described by a discrete contact model (DCM), which is formulated as a constrained least-squares optimization statement: the velocity field is seeked as the projection of the spontaneous velocities of each particle into a feasibility set (which prevents the overlap between particles and between particles and obstacles). The parametric variations in the problem are associated to the geometric configuration of the system and to the initial positions of the particles: they have a dramatic impact in the solution, both in terms of particles positions and contact forces. We investigate new developments of the reduced-basis method and supervised machine-learning techniques to effectively find, in a decorrelated manner, primal and dual reduced spaces. We perform a non-linear reconstruction from the first coordinates of a linear reduced basis approximation, in order to achieve a better performance than the linear reconstruction. To assess the validity of the method, the nonlinear compressive strategy is then compared to more standard linear and nonlinear approximations. Maury, B., Venel, J. (2011). A discrete contact model for crowd motion. ESAIM: Mathematical Modelling and Numerical Analysis, 45(1), 145-168.

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MS173

Dynamical Low Rank Approximation of SDEs

The Dynamical Low Rank Approximation (DLRA) technique is a type of time-dependent reduced-order model that has been applied in various application fields with appealing results for computational time and accuracy. The fact that makes this method very attractive in uncertainty quantification problems, such as random PDEs, is that in DLRA the solution is composed of time-dependent deterministic and stochastic bases, allowing the approximation to better track the dynamics of the studied system. Despite being a recent topic, the theoretical and numerical foundation of DLRA for random PDEs is now well-developed, but the same cannot be said for stochastic differential equations (SDEs). In this talk, we present a rigorous mathematical formulation of DLRA for SDEs using the so-called Dynamically Orthogonal (DO) framework. As the DO system of equations is coupled and depends on the inverse of a Gramian, both the existence of solutions and their numerical discretization are not trivial. We will also propose

different first-order schemes of DO for SDEs, showing results of accuracy and highlighting practical advantages and possible drawbacks. Finally, we will illustrate applications of the DO method for SDEs supported by numerical simulations.

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MS174

Scalable Gaussian Processes via Iterative Numerical Methods

Gaussian processes are a powerful nonparametric Bayesian model that have enjoyed widespread usage across a variety of domains like geospatial modeling, inverse problems, Bayesian optimization, and more. However, training and making predictions with Gaussian processes involves computing linear solves, log determinants and associated derivatives of large kernel matrices, resulting in $\mathcal{O}(n^3)$ time and $\mathcal{O}(n^2)$ space complexities for traditional implementations. Circumventing these high computational complexities has historically been done primarily by introducing modelling approximations like conditional independencies that make training and inference significantly more tractable. In this talk, I will discuss prior work that achieves scalability by introducing approximations at the numerical computation level–for example, in how we think about solving linear systems with kernel matrices–rather than at the statistical modelling level. These approximations lead to fast inference and training for a wide variety of Gaussian process models and recently have been shown to have strong theoretical guarantees. Additionally, I will discuss more recent ongoing work that seeks to bridge the final remaining gap between GPs trained using these new numerical approximation methods and GPs trained using more classic approximate inference techniques: the ability to train while considering only subsets of data at a time.

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MS174

Scalably and Directly Fitting Spectral Densities of Gaussian Processes Measured at Fully Irregular Locations

Provably valid spectral densities are significantly easier to specify than covariance functions. For measurements made on regular grids, tooling exists for practitioners to work primarily in the spectral domain and exploit the additional flexibility in modeling that it affords them. But for data measured at irregular locations, the options for spectral domain modeling are limited and often do not permit the use of likelihoods for estimation. In this work, we present a framework that allows one to write models for spectral densities and fit them with likelihood-based methods even for data that have been measured at fully irregular locations and spectral densities that decay very slowly, like Matérn(1/2) models. Because our method provides the covariance function at arbitrary locations, it can also be used within the many frameworks for scalably approximating Gaussian log-likelihoods, which we demonstrate with an application using Vecchia's approximation.

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MS174

Gaussian Process Modeling for Inverse Problems: State of Play

Gaussian processes (GPs) provide a powerful set of principled modeling methods that have enjoyed enduring popularity among researchers on uncertainty quantification, machine learning, and statistical modeling of data. GPs are useful tools for the solution of inverse problems, and play a key role in spatial/space-time modeling, climate data analysis, Bayesian black-box function optimization, simulation-model verification and validation, and design of computer experiments, among many other applications. In recent years, GP modeling has entered its own Big Data phase, as new accurate approximation methods that abate the $\mathcal{O}(N^3)$ complexity scaling have been formulated and implemented in software libraries. These developments have favored rapid growth of GP applications for the solution of inverse problems. Current research trends include new applications to climate data analysis and modeling that exploit novel scaling methods, metamodel development for design and analysis of computer model experiments, methods for GP model validation and iterative improvement, and new scalable GP approximations that complement or improve upon existing fast kernel methods. I will review the state-of-play of this research, to set the stage for the talks that will follow in the 4 sessions of this Minisymposium.

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MS174

Exact Gaussian Processes for Massive Datasets via Non-Stationary Sparsity-Discovering Kernels

A Gaussian Process (GP) is a prominent mathematical framework for stochastic function approximation in science and engineering applications. Its success is largely attributed to the GPs analytical tractability, robustness, and natural inclusion of uncertainty quantification. Un-

fortunately, the use of exact GPs is prohibitively expensive for large datasets due to their unfavorable numerical complexity. Existing methods addressing this issue utilize some form of approximation usually considering subsets of the dataset or finding representative pseudo-points that render the covariance matrix well-structured and sparse. These approximate methods can lead to inaccuracies and often limit the users flexibility in designing expressive kernels. Instead of inducing sparsity via data-point structure, this talk shows how to take advantage of naturally occurring sparsity by allowing the kernel to discover instead of induce sparse structure. The premise of this work is that the datasets and physical processes modeled by GPs often exhibit natural sparsities, but commonly used kernels do not allow us to exploit such sparsity. The core concept of exact, and at the same time sparse GPs relies on kernel definitions that provide enough flexibility to learn and encode not only non-zero but also zero covariances. This principle of ultra-flexible, compactly-supported, and non-stationary kernels, combined with HPC, lets us scale exact GPs well beyond 5 million data points.

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MS175

Learning Directed Graphical Models

Data-informed structured probabilistic models are typically used to model complex probability distributions and are built by expert knowledge and available data. Such models are commonly formulated as Probabilistic graphical models (PGMs). In this talk, we focus on learning structure and parameters PGMs with causal relationships between model components via optimal transport methods. Such models are also known as Bayesian networks and are PGMs with directed acyclic graphical structure. We present learning methods by taking advantage of monotone triangular transport maps and we demonstrate our results on examples with both noisy linear and nonlinear dependencies between model components.

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MS175

Nonlinear Causal Discovery by Score Matching

Probabilistic graphical models are a powerful tool for representing conditional (in)dependence assumptions of a joint distribution. Unfortunately, the bitter lesson of causality is that correlation doesnt mean causation, which is why they are unsuitable for tasks involving causal reasoning. In contrast, the formalism of Structural Causal Models encodes assumptions about the causal relationships between a system of variables. If the model is expressive enough, joint observations of X and Y can tell whether X causes Y or Y causes X: the inference task of mapping the distribution p(X, Y) to the corresponding causal model is known as causal discovery. In this talk, we start from the observations that traditional methods for causal discovery are fundamentally limited by their computational demand, which prevents scaling inference to systems of many variables. We will present contributions towards tackling these challenges in the case in which the gradient of the log-likelihood, i.e. the score function of the data, is known. Indeed, we show that efficient estimation of the score function by score matching techniques unlocks causal discovery in high dimensions, with theoretical guarantees of identifiability of the model.

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MS175

Multi-View Causal Representation Learning with Partial Observability

We present a unified framework for studying the identifiability of representations learned from simultaneously observed views, such as different data modalities. We allow a partially observed setting in which each view constitutes a nonlinear mixture of a subset of underlying latent variables, which can be causally related. We prove that the information shared across all subsets of any number of views can be learned up to a smooth bijection using contrastive learning and a single encoder per view. We also provide graphical criteria indicating which latent variables can be identified through a simple set of rules, which we refer to as identifiability algebra. Our general framework and theoretical results unify and extend several previous work on multi-view

nonlinear ICA, disentanglement, and causal representation learning. We experimentally validate our claims on numerical, image, and multi-modal data sets. Further, we demonstrate that the performance of prior methods is recovered in different special cases of our setup. Overall, we find that access to multiple partial views offers unique opportunities for identifiable representation learning, enabling the discovery of latent structures from purely observational data.

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MS176

P-th Root of Stochastic Matrices: a Deep Unsupervised Learning Approach

Transition matrices are a tool used to describe the transition probabilities of a Markovian process. From an applied perspective, transition matrices are, for example, used in the fields of credit risk management and the study of chronic diseases. In these domains, it is possible to estimate annual transition probabilities, but for modeling purposes, it may be necessary to calculate transition matrices for shorter and more restricted time intervals. From a mathematical viewpoint, when assuming an homogeneous Markov chain, this requirement translates into calculating the p-th root of a stochastic matrix through a constrained optimization problem. In this talk, we will present the results related to a novel approach based on the use of a neural network trained through an unsupervised learning process. Specifically, this approach will be compared with iterative algorithms already presented in the literature used to solve this problem.

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MS176

Accelerating the Development of Novel RD Technologies for Achieving Net-Zero Emissions: An Optimal Experimental Design Approach

The challenge to combat climate change demands a profound shift in the energy sector to pursuit net-zero emissions. This transformation requires a transition from fossil fuel-based energy to renewable and low-carbon alternatives. Embracing renewable energy technologies, including biotech, solar, wind, hydro, and geothermal power, stands as a pivotal strategy to reduce carbon emissions. For instance, carbon capture, utilization, and storage (CCUS) technologies and biofuels play critical roles in mitigating emissions across power generation, industry, and transportation sectors. This transition towards sustainability demands collaborative efforts, innovative solutions, and supportive policies. However, technological advancements often rely on time-consuming and cost-intensive experimental campaigns. To address this effort, Optimal Experimental Design (OED) techniques offer an optimization path. OED expedites the transfer of experimental results into industrial solutions adhering to quality, safety standards, and design constraints. By identifying input-output relationships, OED minimizes the number of required experimental trials. Notably, when combined with machine learning, OED can iteratively adapt experiments based on initial outcomes, improving models and reducing uncertainty, ultimately leading to better decision-making and more accurate predictions. In this workshop, the results of the application of OED for accelerating novel RD technologies is shown.

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MS177

Real-Time Bayesian Inversion of Autonomous Systems with Application to Tsunami Forecasting

Hessian-based algorithms for the solution to Bayesian inverse problems typically require many actions of the Hessian matrix on a vector. For problems with high-dimensional parameter fields or expensive-to-evaluate forward operators, a direct approach is often computationally intractable, especially in the context of real-time inversion. One way to overcome the computational bottleneck of Hessian matrix-vector multiplications in these large-scale inverse problems is to exploit the structure of the underlying operators. A particular class of operators for which we can exploit the structure very effectively are those representing autonomous systems. The evolution of such systems with respect to any given input may depend on the systems current state but does not explicitly depend on the independent variable (e.g., time). We present a scalable and computationally efficient approach for Bayesian inversion of problems involving autonomous systems. Our approach splits the computation into a precomputation ("offline") phase and a real-time inversion ("online") phase. Contrary to other methods, this approach does not employ a lower-fidelity approximation but instead uses the full discretization obtained from the PDE-based model. The method is applied to a real-time tsunami Bayesian inverse problem involving a time-invariant dynamical system. Scalability and efficiency of the implementation are demonstrated for state-of-the-art GPU-accelerated compute architectures.

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MS177

Normalizing Flows for Bayesian Experimental Design in Imaging Applications

Neural density estimators such as normalizing flows have shown promise for estimation of the Bayesian posterior in a variety of imaging problems. Few works have explored how to practically exploit the probabilistic information contained in the full Bayesian solution of the inverse problem. Here we explore a simple modification to conditional normalizing flow training that enables Bayesian experimental design without modifying existing architectures. Based on a relationship between the expected information gain and maximum-likelihood training of normalizing flows, we show that experimental design can be achieved with the same training objective. We first verify that our method maximizes the expected information gain using a stylized problem. Then, we demonstrate our method can solve imaging problems in large scale medical and seismic applications.

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MS177

Hyper-Differential Sensitivity Analysis for Large Scale Inversion

Hyper-Differential Sensitivity Analysis (HDSA) with respect to model-discrepancy is used to update approximate optimization solutions that emulate higher-fidelity, physics-based optimization solutions by incorporating data from the high-fidelity physics. This approach avoids intrusive implementations and only depends on small number of forward evaluations of the higher-fidelity models. In this presentation, we investigate strategic sampling algorithms using optimal experimental design concepts combined with HDSA and Bayesian theory to reduce the error between the lower and higher-fidelity optimization solutions. We demonstrate our approach on various PDE exemplars and show improvements over random sampling.

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MS178

Model Reduction Without sScale Separation

Reduced models of complex nonlinear dynamic phenomena are of interest for many reasons: they reduce computational cost, offer insights into mechanisms, and enable mathematical analysis. Recent advances in machine learning have energized research in data-driven model reduction methods. In this overview, I will highlight some of the many issues that arise in model reduction and data-driven modeling and touch on some useful conceptual frameworks and dynamical ideas, focusing in particular on those relevant to the talks in this minisymposium.

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MS178

Modeling Extreme Events and Intermittency in Turbulent Diffusion Models

Transport-dominated phenomena represents a major challenge for reduction methods and uncertainty quantification, primarily due to the presence of nonlinear coherent wave structures. In this talk we delve into a simplified model for turbulent diffusion that features intermittency and extreme events that arise due to resonance. We discuss the tracers explicit statistical solutions, revealing non-Gaussian extreme events, and numerical simulations that display the various regimes of intermittency inherent in such models. The model also permits extension to large deviations techniques, which we also explore, and serves as a test model for various other efforts in uncertainty quantification, including data assimilation and scientific machine learning.

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MS178

An Efficient Data-Driven Multiscale Stochastic Reduced Order Modeling Framework for Complex Systems

In this paper, a systematic multiscale stochastic ROM framework is developed for complex systems with strong chaotic or turbulent behavior. The new ROMs fundamentally differ from the traditional Galerkin ROM (G-ROM) or those deterministic closure ROMs that aim to minimize path-wise errors and apply mainly to laminar systems. At the same time, it also exploits cheap but effective conditionally linear functions as the closure terms to capture the statistical features of the medium-scale variables and their feedback to the large scales. In addition, physics constraints of energy-conserving nonlinearities are incorporated into the new ROM. One unique feature of the resulting ROM is that it facilitates an efficient and accurate scheme for nonlinear data assimilation, the solution of which is provided by closed analytic formulae that do not require ensemble methods. It allows the new ROM to avoid many potential numerical and sampling issues in recovering the unobserved states from partial observations. The closure term calibration is efficient and systematic via explicit mathematical formulae. The new ROM framework is applied to complex nonlinear systems. The out-of-sample numerical results show that the new ROM significantly outperforms the G-ROM in both scenarios regarding reproducing the dynamical and statistical features and recovering unobserved states via the efficient data assimilation scheme.

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MS179

TBD

MS180

The UQTk C++/Python Toolkit for Uncertainty Quantification: Overview and Applications

The UQ Toolkit (UQTk) is a collection of libraries, tools and apps for the quantification of uncertainty in numerical model predictions. As one of the software tools offered by the DOE SciDAC FASTMath Institute, UQTk offers intrusive and non-intrusive methods for forward uncertainty propagation, tools for sensitivity analysis, sparse surrogate construction, low-rank-tensor approximations, Bayesian inference via various flavors of MCMC, model error assessment, as well as several other capabilities. The core libraries are implemented in C++ but a Python interface is available for easy prototyping and incorporation in UQ workflows. The talk will give an overview of UQTk capabilities and illustrate its application to representative scientific workflows.

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MS180

Lagun : An Open Source Platform for Data Exploration and Optimization

Lagun is an open-source platform dedicated to the exploration and analysis of small datasets, collected from experiments or expensive simulation models. Intended for non-expert users in computer experiments and uncertainty quantification, it is coded in R shiny to provide an interactive and user-friendly interface. The user is guided step-by-step through workflows to apply safely the different methodologies, which are : (i) Building optimized designs of experiments in order to generate a relevant dataset

(good spatial repartition in the input space) (ii) Many visualization tools to explore datasets and have a first overview of the input–output relationship (main trends, which input is more influent...) (iii) Build surrogate models to predict approximatively and quickly the output for a new value of the inputs. Different types of surrogate models are proposed (iv) The surrogate models can then be exploited intensively to perform uncertainty quantification, sensitivity analysis, optimization (deterministic/under uncertainty, mono/bi objective, under constraints or not) (v) Lagun can be directly connected with simulation scripts, to perform sequential optimization, calibration of numerical simulations etc. Lagun uses state-of-the-art methodologies that are provided by members of the UQ community or that results from the Safran-IFPEN collaborative project

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MS180

A Unified Benchmarking Platform for UQ Algorithms in UQLab

Thorough validation and benchmarking against the state-of-the-art are critical components in the development of novel algorithms and tools. Nevertheless, the comprehensive performance comparison between different solutions to the same problem is still sparse in the literature, mostly relegated to dedicated review studies rather than a standard practice. This is especially noticeable in the field of uncertainty quantification, where algorithm performance is also strongly affected by repeatability, finite computational resources and the wide range of possible application fields. We introduce the in-development benchmark module for the UQLab platform, a novel toolbox that enables thorough, standardized benchmarking facilities to ease the cumbersome process of placing the performance of a new algorithm in the rich landscape of possible alternatives putational models with uncertain parameters

- Competitors, which include different sets of algorithms to be compared against one another
- Performance measures, allowing users to compare and rank the performance of each competitor quantitatively.

Additionally, the benchmark module comes with an extensive pre-calculated library of benchmarks and case studies based on current literature and our own experience.

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MS180

Sparse Grids with SG++ for UQ and Hierarchical Bayesian Optimization

Adaptive sparse grids provide a flexible and versatile way to represent higher-dimensional dependencies. We present recent developments of and with SG^{++}, the most extensive software toolkit for spatially adaptive sparse grids. It is a multi-platform toolkit with fast and efficient algorithms. In the context of UQ, it provides sparse grid functionality for forward propagation, model calibration, optimization, density estimation, and more. It furthermore provides state-of-the-art not-a-knot B-spline ansatz functions with beneficial properties. For example, derivatives are directly available without the need for numerical approximations. We discuss properties of SG^{++} and present its use for the quantification of uncertainties for parameter estimation of an industrial electric motor using hierarchical Bayesian inversion.

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MS181

Sampling in Unit Time with Kernel Fisher-Rao Flow

We introduce a new mean-field ODE and corresponding interacting particle systems for sampling from an unnormalized target density or Bayesian posterior. The interacting particle systems are gradient-free, available in closed form, and only require the ability to sample from the reference density and compute the (unnormalized) target-to-reference density ratio. The mean-field ODE is obtained by solving a Poisson equation for a velocity field which will transport samples along the geometric mixture of the two densities, which is the path of a particular Fisher–Rao gradient flow. We employ a reproducing kernel Hilbert space ansatz for the velocity field, which makes the Poisson equation tractable and enables us to discretize the resulting mean-field ODE over finite samples as a simple interacting particle system. The mean-field ODE can be additionally be derived from a discrete-time perspective as the limit of successive linearizations of the Monge-Ampere equations within a framework known as sample-driven optimal transport. We demonstrate empirically that our interacting particle systems can produce high-quality samples in test problems with varying characteristics.

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MS181

Manifold Learning in the Wasserstein Space

In this talk, we introduce LOT Wassmap, a computationally feasible algorithm to uncover low-dimensional structures in the Wasserstein space. The algorithm is motivated by the observation that many datasets are naturally interpreted as probability measures rather than points in $\mathbb{R}^n$, and that finding low-dimensional descriptions of such datasets requires manifold learning algorithms in the Wasserstein space. Most available algorithms are based on computing the pairwise Wasserstein distance matrix, which can be computationally challenging for large datasets in high dimensions. Our algorithm leverages approximation schemes such as Sinkhorn distances and linearized optimal transport to speed-up computations, and in particular, avoids computing a pairwise distance matrix. Experiments demonstrate that LOT Wassmap attains correct embeddings and that the quality improves with increased sample size. We also show how LOT Wassmap significantly reduces the computational cost when compared to algorithms that depend on pairwise distance computations.

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MS181

Algorithms for mean-field variational inference via polyhedral optimization in the Wasserstein space

We develop a theory of finite-dimensional polyhedral subsets over the Wasserstein space and optimization of functionals over them via first-order methods. Our main application is to the problem of mean-field variational inference, which seeks to approximate a distribution π over $\mathbb{R}^d$ by a product measure $\pi^\star$. When π is strongly log-concave and log-smooth, we provide (1) approximation rates certifying that $\pi^\star$ is close to the minimizer $\pi^\star_\diamond$ of the KL divergence over a *polyhedral* set $\mathcal{P}_\diamond$, and (2) an algorithm for minimizing $\mathrm{KL}(\cdot\|\pi)$ over $\mathcal{P}_\diamond$ with accelerated complexity $O(\sqrt{\kappa}\log(\kappa d/\varepsilon^2))$, where κ is the condition number of π. Joint with Yiheng Jiang (NYU) and Sinho Chewi (IAS).

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MS181

A Mean-Field Games Laboratory for Generative Modeling

We demonstrate the versatility of mean-field games (MFGs) as a mathematical framework for explaining, enhancing, and designing generative models. We establish connections between MFGs and major classes of flow and diffusion-based generative models by deriving continuous-time normalizing flows, score-based models, and Wasserstein gradient flows through different choices of particle dynamics and cost functions. Furthermore, we study the mathematical structure and properties of each generative model by examining their associated MFG's optimality condition, which consist of a set of coupled forward-backward nonlinear partial differential equations. The optimality conditions of MFGs also allow us to introduce HJB regularizers for enhanced training of a broad class of generative models. We present this framework as an MFG laboratory which serves as a platform for revealing new avenues of experimentation and invention of generative models.

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MS182

Bayesian Nonparametric Methods for Low Frequency Diffusion Data

The talk will consider Bayesian nonparametric inference in multi-dimensional diffusion models from low-frequency data. Implementation and analysis of Bayesian procedures

in such setting is a notoriously delicate task due to the involved likelihood structure. We propose novel algorithms based on the underlying PDE characterisation of the transition densities. This approach allows the numerical evaluation of the likelihood via standard numerical methods for elliptic PDEs, providing the basis for the construction of a random-walk-type MCMC algorithm for posterior inference with Gaussian process priors. Furthermore, using PDE perturbation arguments, we characterise the likelihood gradient, which we use to implement Langevin-type MCMC samplers as well as optimisation methods for the computation of the maximum-a-posteriori estimates. Joint work with Sven Wang (Humboldt University Berlin).

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MS182

Advanced Monte Carlo Methods in the Context of Bayesian Inference

We consider the problem of estimating expectations with respect to a target distribution with unknown normalizing constant, and where even the unnormalized target needs to be approximated at finite resolution. Under such an assumption, we extend a recently introduced multi-index Sequential Monte Carlo (SMC) ratio estimator, which provably enjoys the complexity improvements of multi-index Monte Carlo (MIMC) and the efficiency of SMC for inference. The present work leverages a randomization strategy to remove bias entirely, which simplifies estimation substantially, particularly in a MIMC context, where the choice of index set is otherwise important. With theoretical results, the proposed method provably achieves the same canonical complexity of MSE^{-1} under appropriate assumptions as the original method, but without discretization bias. It is illustrated on examples of Bayesian inverse problems. If time permits I will talk about the work on the parallelization of SMC and applications of related methods to Bayesian neural networks.

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MS182

A General Involution Framework for MCMC Algorithms and Applications to Bayesian Inverse Problems

We consider a general framework for Metropolis-Hastings algorithms used to sample from a given target distribution on general state spaces. Our framework is based on a fundamental involution structure, and shown to encompass several popular algorithms as special cases, both in the finite- and infinite-dimensional settings. In particular, random walk, preconditioned Crank-Nicolson (pCN), schemes based on a suitable Langevin dynamics such as the Metropolis Adjusted Langevin algorithm (MALA), and also ones based on Hamiltonian dynamics including several variants of the Hamiltonian Monte Carlo (HMC) algorithm. In addition, we provide an abstract framework for algorithms that generate multiple proposals at each iteration, which yield efficient sampling schemes through the use of modern parallel computing resources. Here we derive several generalizations of the aforementioned algorithms following as special cases of this multiproposal framework. To illustrate effectiveness of these sampling procedures, we present applications in the context of some Bayesian inverse problems in fluid dynamics. This is based on joint works with N. Glatt-Holtz (Tulane), A. Holbrook (UCLA), and J. Krometis (Virginia Tech).

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MS183

A Deep Learning Method for Filtering in the Stochastic Reaction Networks Setting for Continuous-Time and Noise-Free Observations

Recent advances in fluorescence and microscopy have enhanced single-cell studies in systems and synthetic biology. Nevertheless, the simultaneous tracking of multiple molecular species remains constrained by the limited number of available fluorescent wavelengths. As a consequence, researchers often resort to estimating the behaviour of unobserved species, introducing a complex stochastic filtering problem to infer hidden dynamics. In this work, we introduce a novel deep learning approach tailored to address this challenge, particularly for continuous-time, noise-free observations. Using a piecewise deterministic Markov process and martingale representation, we employ a deep neural network trained with Monte-Carlo simulations to efficiently solve the filtering equation. This approach performs favourably in comparison to traditional particle filtering methods, offering a quicker and more efficient way to analyse and possibly control single-cell dynamics.

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MS183

A Divide-and-Conquer Approach for Analyzing High-Dimensional Stochastic Reaction Network System

Intracellular gene expression systems are inevitably random due to low molecular counts. Central to the analysis and inference of such systems is solving the Chemical Master Equation (CME), which characterizes the probability evolution of the randomly evolving copy-numbers of the reacting species. While conventional methods such as Monte-Carlo simulations and finite state projections exist for estimating CME solutions, they suffer from the curse of dimensionality, significantly decreasing their efficacy for high-dimensional systems. Here, we propose a new computational method that resolves this issue through the divide-and-conquer idea. Our method divides the system into a leader system and several conditionally independent follower subsystems. The solution of the CME is then constructed by combining Monte Carlo estimation for the leader system with stochastic filtering procedures for the follower subsystems. We develop an optimized system decomposition, which ensures the low-dimensionality of the sub-problems, thereby allowing for improved scalability with increasing system dimension. The efficiency and accuracy of the method are demonstrated through several biologically relevant computational examples in high-dimensional estimation and inference problems. Also, we show that our method can successfully identify a yeast transcription system at the single-cell resolution, leveraging time-course data. This demonstrates the efficacy of our approach in practical applications.

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MS183

Particle Filters for State Estimation of Stochastic Reaction Networks from Exact Partial State Observations

Stochastic reaction network models are an accurate representation of intra-cellular chemical reactions and are fundamental in the study of systems biology. These models form a class of continuous time Markov chains with a multidimensional non-negative integer lattice as state space. In addition to chemical reactions, these models are applicable in other forms population processes such as predator-prey systems and epidemiological models (SEIR) etc. We describe new particle filter methods for the estimation of unobserved states and parameters of a stochastic reaction network based on exact partial state observations. We consider two scenarios, one in which the observations are made continuously in time over a window and the other in which observations are made in snapshots of time. We provide derivations of our methods as well as numerical examples that illustrate the applicability of our approach.

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MS184

Filtering Dynamical Systems Using Observations of Statistics

We consider the problem of filtering dynamical systems, possibly stochastic, using observations of statistics. Thus the computational task is to estimate a time-evolving density $\rho(v,t)$ given noisy observations of ρ; this contrasts with the standard filtering problem based on observations of the state v. The task is naturally formulated as an infinite-dimensional filtering problem in the space of densities ρ. However, for the purposes of tractability, we seek algorithms in state space; specifically we introduce a mean field state space model and, using interacting particle system approximations to this model, we propose an ensemble method. We refer to the resulting methodology as the ensemble FokkerPlanck filter (EnFPF). Under certain restrictive assumptions we show that the EnFPF approximates the KalmanBucy filter for the FokkerPlanck equation, which is the exact solution of the infinite-dimensional filtering problem; our numerical experiments show that the methodology is useful beyond this restrictive setting. Specifically the experiments show that the EnFPF is able to correct ensemble statistics, to accelerate convergence to the invariant density for autonomous systems, and to accelerate convergence to time-dependent invariant densities for non-autonomous systems. We discuss possible applications of the EnFPF to climate ensembles and to turbulence modelling.

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MS184

Factorization-Based Online Variational Inference

for Parameter-State Estimation

Online inference considers simultaneously estimating the parameters and states of a system as the system is evolving. This procedure is a crucial and challenging task in many application areas such as robotics and weather prediction. In this talk, we introduce a simple and flexible online variational inference method for parameter-state estimation. Our method provides an approximate joint posterior distribution of system parameters and current states at every time step by assimilating data incrementally. It is based on a particular factorization of the approximate joint posterior, which enables our method to avoid assumptions of the joint posterior structure. The marginal distribution over parameters can be learnt using an arbitrary representation family. Moreover, the functional representation of hyper-parameters for the variational distribution of current state given parameters can be chosen to fulfill the requirements of speed or performance. This facilitates our method to provide an accurate approximation to the joint posterior in a flexible way. For linear systems, only the marginal variational distribution of parameters needs to be optimized when maximizing the ELBO. The filtering distributions given parameters are Gaussian distributions, of which the mean and covariance are approximated as functions of parameters recursively. The effectiveness of the proposed method is illustrated by applications on low- and high-dimensional, partially observable dynamical systems.

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MS184

An Adaptive Ensemble Filter for Heavy-Tailed Distributions

Heavy tails is a common feature of filtering distributions that results from the nonlinearity and stochasticity of the dynamical and observation processes. In these settings, the Kalman filter and its ensemble version - the ensemble Kalman filter (EnKF) - designed under Gaussian assumptions have degraded performance. t-distributions are a parametric family of distributions whose tail-heaviness is modulated by a degree of freedom ν interpolating between a Cauchy distribution for $\nu = 1$ and a Gaussian distribution for $\nu = \infty$. Leveraging ideas from measure transport (Spantini et al., SIAM Review, 2022), we present a generalization of the EnKF whose prior-to-posterior update $\boldsymbol{T}$ leads to exact inference for t-distributions. The map $\boldsymbol{T}$ is parameterized by the statistics of the joint t-distribution of the states and observations. For nonlinear state-space models, we use a $l1$-regularized expectation-maximization (EM) algorithm (Finegold and Drton, arXiv preprint, 2014) to estimate $\boldsymbol{T}$ from joint samples. This new filter features an intrinsic adaptive multiplicative inflation, and an adaptive localization due to the $\ell 1$-penalization in the EM algorithm. By sequentially estimating the degree of freedom, our filter can automatically adapt its prior-to-posterior update to the tail-heaviness of the data. We assess this new ensemble filter on challenging settings.

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MS184

A Bayesian Framework for Uncertainty Quantification in Dynamical Systems in the Presence of Corrupted Measurements

We will present a Bayesian framework that aims to advance the state-of-the-art of forecasting dynamical systems in the presence of corrupted data. This framework will rely on data fusion algorithms that estimate the effects of corruption, and mitigate their impact on predictions. The framework employs a hidden Markov model to incorporate the impact of parameter, model, and measurement uncertainty on the system dynamics operator, as well as components resulting from measurement corruption. We will demonstrate the framework on canonical dynamical systems and on 3DOF models associated with re-entry vehicles. We will compare the performance of this approach when employing Markov Chain Monte Carlo methods to sample the joint posterior distribution of the parameter space with approximate but cheaper descriptions of the high-dimensional posterior distribution obtained using variational inference. This framework will impact the estimation of corruption incident to a navigation system, such as GPS spoofing.

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MS185

Utilizing Data-Driven Models to Enable Error Es-

timation for Surrogate Models

In recent years, data-driven and machine learning methods have become much more prevalent in computational science, largely due to their ability to learn and exploit low-dimensional structure in high-dimensional data. In this presentation, we will describe some of our recent work on using data-compression methods to detect and exploit low-dimensional latent structure to enable the accurate and efficient computation of adjoint-based a posteriori error estimates for surrogate models based on either traditional response surface methods, e.g., sparse grids, or based on data-driven models. This recent work alleviates some of the computational challenges in some of our previous work on this topic and expands the applicability of this approach. Theoretical results will be presented to validate the trustworthiness and robustness of the approach and numerical results will also be present for transient nonlinear multiphysics applications.

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MS186

Uncertainties in Data-Driven Climate Predictions

Deep learning is a tool that is increasingly being leveraged by the earth system modeling community due its capacity to ingest large quantities of data to discover patterns and relationships, incorporate limited observed data, and make enhanced, faster data-driven earth-system predictions. When using earth-system models directly to make predictions, the various sources of uncertainties can be quantified, e.g. the distinction between internal variability and model uncertainty. However, when we instead make enhanced predictions with data-driven models, a further source of uncertainty is introduced by the data-driven system, and we also must ensure that the other sources of uncertainty are properly accounted for and quantified when making a prediction with such models. This becomes especially important in the case of impacts assessments where decisions are routinely required to be made under uncertainty. In this talk, I will present our recent efforts to quantify the various sources of uncertainty in our predictions of climate quantities from data-driven models. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and is supported by LLNL Laboratory Directed Research and Development project 22-SI-008.

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MS186

A Hybrid Machine Learning Climate Simulation Using High Resolution Convection Modelling

Underrepresentation of cloud formation is a known failing in current Climate simulations. The coarse grid resolution required by the computational constraint of integrating over long time scales does not permit the inclusion of underlying cloud generating physical processes. This work employs a multi-output Gaussian Process (MOGP) trained on high resolution Unified Model (UM) simulation data to predict the variability of temperature and specific humidity fields within the climate model. A proof-of-concept study has been carried out where a trained MOGP model is coupled in-situ with a simplified Atmospheric General Circulation Model (AGCM) named SPEEDY. The temperature and specific humidity profiles of the SPEEDY model outputs are perturbed at each timestep according to the predicted high resolution informed variability. 10-year forecasts are generated for both default SPEEDY and ML-hybrid SPEEDY models and output fields are compared ensuring hybrid model predictions remain representative of Earth's atmosphere. Some changes in the precipitation, outgoing longwave and shortwave radiation patterns are observed indicating modelling improvements in the complex region surrounding India and the Indian sea.

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MS186

Flexible Emulation for Hydroclimate Scenarios with Bayesian Transport Maps

Uncertainty quantification for climate impacts on the global hydrological cycle relies on credible representation of the probability distribution of multiple quantities of interest. These variables capture processes operating at a range of spatio-temporal scales that are represented in multiple components of modern Earth-system models. Under suitable experimental designs, ensembles of model runs provide information on the distributions of interest, but computing and storage resources often limit the ensemble sizes. This work demonstrates an emulation capability through Bayesian transport maps (BTM) that enables fast unconditional and conditional sampling from a spatio-temporal model trained on a modest-sized collection of geophysical model runs. The approach is implemented for hydrologic variables from an ensemble of land-surface model (LSM) experiments that is assembled from perturbed initial and boundary conditions. Probabilistic assessments for snow timing and extent under contemporary and future climate scenarios are illustrated with the BTM approach.

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MS186

Development and Calibration of the Arctic Coastal Erosion (ACE) Model, Towards Uncertainty Quantification of Climate Change-Induced Arctic Permafrost Degradation

Although the Arctic is warming at a rate of 4x the rest of the globe, current tools for quantifying permafrost erosion fail to explain the episodic, storm-driven erosion events occurring in the region. This talk will describe the development and calibration of a new thermo-mechanics-based ACE (Arctic Coastal Erosion) model for the simulation of permafrost erosion off the Arctic coast of Alaska, towards enabling UQ of climate change-induced Arctic permafrost degradation. The ACE model has several unique characteristics, including: (1) the ability to predict failure from any allowable deformation (block failure, thermo-denudation, thermo-abrasion); (2) the ability to predict failure modes from constitutive (rather than empirical) relationships; (3) the capability to remove elements from the underlying finite element mesh based on specified erosion criteria; and (4) the incorporation of realistic oceanic and atmospheric boundary conditions obtained from stand-alone oceanic simulations and observational data, respectively. Following a description of the key features of ACE, I will present some results generated using this model, namely: (1) results from a sensitivity study performed using the model run in mechanics-only mode, and (2) results demonstrating that the model is capable of reproducing erosion behavior observed during a summer/fall 2018 field campaign at Drew Point, Alaska. I will also discuss perspectives towards deploying the model in forward UQ analyses.

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MS187

Automated Deep Neural Network Ensembles for Uncertainty Quantification in Scientific Machine Learning

Data-driven deep learning-based models have exhibited significant gains in accuracy and time-to-solution over classical methods. However, the widespread adoption of deep learning models remains limited due to their inherent black-box nature, which lacks trustworthiness. We present a unified strategy that efficiently discovers high-performing deep learning models by utilizing distributed computing for scientific machine learning tasks, while quantifying epistemic and aleatoric uncertainties. For uncertainty quantification, we employ a variance decomposition approach that separates aleatoric and epistemic uncertainty components, thereby enhancing the interpretability of the uncertainty estimates. We validate our proposed approach using real-world, high-dimensional scientific machine learning problems with complex dynamics. Through extensive experimentation and validation, our integrated automated deep ensemble approach showcases its efficacy in accurately predicting complex systems and providing reliable uncertainty estimates.

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MS187

Neural Networks Ensembles to Accelerate Power Grid Contingency Analysis

This talk presents an application of Bayesian Graph Neural Networks for power grid contingency analysis. Contingency analysis aims at modeling potential outages in specific elements of the grid such as failure of transmission line(s) or generator(s) and evaluate their effect on the performance of the power system overall, to help guide post-outage response. Contingency analysis is important to evaluate power system security and reliability, especially with the growing integration of renewable energy sources, which depend on external factors such as weather and are less predictable. Contingency analysis requires solving computationally expensive nonlinear power flow simulation for all possible contingencies of interest. This high computational cost hinders contingency analysis for higher-order contingencies (loss of multiple components) for large enough grids. Efficient machine learning (ML) algorithms such as neural networks (NNs) can be leveraged as surrogate of these expensive power flow solvers. However, for

such high-consequence application, it is critical to design ML algorithms that are both accurate and embed uncertainty quantification to allow a reliable assessment of our confidence in their predictions. In this talk, we will present some results on the application of Bayesian graph NNs that can 1) integrate knowledge about the grid topology to improve accuracy for out-of-distribution predictions and 2) quantify uncertainties in predictions via ensembling.

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MS187

Coupling Bayesian Recurrent Neural Networks and State-Space Models Through Analytically Tractable Inference

In their original form, long short-term memory (LSTM) neural networks (NN) are deterministic models which consider their parameters as having deterministic values, hence failing to account for the epistemic uncertainties. By contrast, Bayesian LSTMs consider this epistemic uncertainty by placing a distribution over the parameters. Variational inference is a common method used to create Bayesian LSTMs. However, it relies on gradient descent and backpropagation for inferring the parameters, and it is thus not compatible with close-form probabilistic methods such as state-space models. The Tractable Approximate Gaussian Inference (TAGI) method allows performing analytical Bayesian inference in NNs. In this work, we present the mathematical formulations for using the TAGI method with the LSTM architecture for obtaining analytically the posterior mean vectors and diagonal covariance matrices for the LSTM's parameters and hidden states. We show through experimental comparisons that our model provides on-par performance compared to the LSTMs trained using backpropagation while enabling to consider the epistemic uncertainty about the model's parameters. This new framework allows to probabilistically couple LSTMs with state-space models because both use Bayesian inference as their learning mechanism. The resulting hybrid model can retain the interpretability feature of SSMs, while exploiting the ability of LSTMs to learn complex patterns automatically with minimal manual setups.

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MS188

Rare Event Simulation Using Multi-Fidelity Importance Sampling and Control Variates with No Model Covariance Requirements

Estimation of small failure probabilities using Monte Carlo is often infeasible for practical, real-world problems due to the high computational cost of evaluating the system response for each sample. Multifidelity modeling is one way to reduce this cost, where accurate but costly high-fidelity model evaluations are replaced with relatively less accurate but cheaper low-fidelity models. In addition, variance reduction methods such as Importance Sampling and Control Variates can be used to reduce the total number of samples necessary for confident failure estimation. We propose a coupled Control Variates and Importance Sampling (CVIS) framework that uses low-fidelity models as the control variate to create a more efficient failure probability estimator. The framework addresses some of the practical challenges of the control variates method by using an estimator for the control variate mean and side-stepping the need to estimate the covariance between the original estimator and the control variate through a creative choice for the tuning constant. Additionally, it allows for a diagnostic that indicates both the efficiency of the algorithm as well as the quality of the control variate. Finally, the performance of the algorithm is explored through analytical examples.

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MS188

Seismic Fragility Analysis of Lifeline Networks Using Subset Simulation

For efficient risk assessment of lifeline systems against earthquakes, various simulation-based and analytical methods have been developed to evaluate the seismic fragility curves of individual structures. However, after an earthquake, network reliability such as two- or k-terminal reliability is critical in efforts to ensure community-level safety. Although various simulation-based methods have been adopted for network reliability analysis owing to their flexibility and scalability, they are quite inefficient for rare network failure events. To address the challenge, this study reformulates the existing binary network limit-state function into more informative piecewise continuous functions for subset simulation (SS). In detail, the proposed functions quantify how close each sample is to the network failure domain, thereby facilitating the construction of intermediate failure events for SS. Constructing a connection between the intermediate failure events and seismic inten-

sity, a single implementation of SS can generate the seismic fragility curve of a lifeline network. The method can be easily extended to evaluate k-out-of-N reliability, which is much more complex than k-terminal reliability. The accuracy and efficiency of the proposed method are tested and demonstrated by several numerical examples.

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MS188

Introducing Efficient Structural Reliability Methods for Stochastic Simulators

Reliability analysis aims at quantifying the probability that uncertainties in the input parameters of a system will lead to performance failure. This process assumes a deterministic performance function, i.e. repeatedly evaluating it with the same set of parameters will consistently yield the same response. Nevertheless, recent literature in uncertainty quantification has started focusing on so-called stochastic simulators. These computational models mimic the stochastic behaviour of systems that exhibit random responses for each set of input parameters. In the context of reliability analysis, it means that a given set of inputs may or may not lead to failure, depending on the uncontrollable latent variability of the model. To explicitly account for this stochasticity, we treat the failure probability as a random variable, which enables deriving meaningful reliability measures, e.g. mean, median, quantiles, etc. Computing these quantities is, of course, possible via Monte Carlo simulation. However, characterising the latent variability of the response in this case requires many calls to the simulator, significantly increasing the already high computational costs of reliability analysis. In this contribution, we propose mitigating the excessive computational costs of simulation-based methods by utilizing stochastic emulators. These are surrogate models for stochastic simulators, and enable computing suitable reliability measures within a feasible computational cost.

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MS188

Physics and Data Co-driven Surrogate mModeling for High-dimensional Rare Event Simulation

In this talk, I will present a physics and data co-driven surrogate modeling framework for efficient rare event simulation of mechanical and civil systems with high-dimensional input uncertainties. The framework embodies a fusion of interpretable low-fidelity physical models with data-driven error corrections. The overarching hypothesis is that a well-designed simplified physical model can extract salient features of the original high-fidelity model, while machine learning techniques can fill the remaining gaps between the surrogate and original models. The coupled physics-data-driven surrogate model is adaptively trained using active learning, aiming to maximize the correlation between the surrogate and original model responses in the critical parametric region for a rare event. Due to the strong correlation between the well-trained surrogate and original models, an importance sampling step is finally introduced to drive the probability estimations toward the theoretically guaranteed solutions. I will present numerical examples of static and dynamic problems with high-dimensional input uncertainties (up to 1,000 input random variables) to demonstrate the proposed framework.

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MS189

Deep Learning Approaches for Extreme Extrapolation in Phase-Field Separation and Metal De-Alloying

Computational simulations of dynamical systems using high-fidelity numerical solvers can be prohibitively expensive for requisite explorations of physical processes of practical interest. In certain application domains, e.g. phase-field modeling, stable simulations require extremely small time-steps which proves to be a bottleneck when the goal is observing physics at long time horizons. To address this issue, we build a deep-learning-based reduced-order-model to extrapolate simulations beyond time horizons achievable with high-fidelity solvers. We employ Fourier Neural Operators (FNOs) and early time step high-fidelity training data to learn an operator capable of skipping time steps when leaping forward in time. We adopt a hybrid auto-regressive approach, with full-order-model time step relaxation interlaced with the FNO evaluations, and operator fine-tuning to control the extrapolation error. We demonstrate this workflow on the Cahn-Hilliard model and phase-field model simulations for liquid metal dealloying.

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MS189

Surrogate Modeling and Data Assimilation with Deep Learning for the Components of the Earth System

Recent studies have shown that it is possible to combine machine learning (ML) with data assimilation (DA) to reconstruct the dynamics of a system that is partially and imperfectly observed. This approach takes advantage of the strengths of both methods. DA is used to estimate the system state from the observations, while ML computes a surrogate model of the dynamical system based on the estimated states. The surrogate model can be defined as an hybrid combination where a physical part based on prior knowledge is enhanced with a statistical part estimated by a neural network. The training of the neural network is usually done offline, once a large enough dataset of model state estimates is available. Online learning has been investigated recently. In this case, the surrogate model is improved each time a new system state estimate is computed. Although online approaches still require a large dataset to achieve a good performance, they naturally fit the sequential framework in geosciences where new observations become available over time. Going even further, we propose to merge the DA and ML steps. This is technically achieved by estimating, at the same time, the system state and the surrogate model parameters. This new method has been applied to low-order models. Preliminary results shows the potential of incorporating DA and ML tightly, and pave the way towards its application to the Integrated Forecast System used for operational Numerical Weather Prediction at ECMWF.

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MS189

An Uncertainty-Aware Digital Twin for Geological Carbon Storage

Arguably, Geological Carbon Storage constitutes the only truly scalable net-negative carbon emission technology. To mitigate its risks and optimize its operations, an uncertainty-aware Digital Twin is being developed. To leverage existing fluid-flow and seismic simulation and imaging capabilities, the envisioned twin combines techniques from sequential and simulation-based Bayesian inference to train its deep generative neural networks to draw samples from the posterior of the Digital Twin's state. Because these samples are conditioned on observed time-lapse field data, these twins are capable of capturing the dynamics of CO_2 plumes and their uncertainty.

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MS189

Digital Twins of Ocean Responses to Climate Change

To better understand the responses of ocean systems to different forcings that represent climate change scenarios, we have explored a wide range of values for the parameters and initial/boundary conditions in an idealized ocean model on a global scale, NeverWorld2, which has intermediate complexity: it incorporates basin-scale geometry for an idealized Atlantic and Southern ocean, with non-uniform ocean depth to allow for mesoscale eddy interactions with topography. The simulation is implemented in Oceananigans.jl, a Julia-based software package for finite volume simulations of the nonhydrostatic Boussinesq equations on CPUs and GPUs. Due to the complexity of global circulation models, however, simulations of ocean processes are prohibitively expensive (even on GPUs), making the tasks of uncertainty quantification for future predictions and sensitivity analysis for model parameters extremely challenging. To address this challenge, we have investigated a wide range of deep learning tools to build dynamical emulators for targeted quantities of interest (QoIs). The efficient emulators will make it possible to capture interactions between the ocean and other components of climate models (e.g., atmospheric models, land models, human activities). This provides valuable scientific information for stakeholders in fighting climate change.

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MS191

Deep Gaussian Process Surrogates for Computer Experiments

Deep Gaussian processes (DGPs) upgrade ordinary GPs through functional composition, in which intermediate GP layers warp the original inputs, providing flexibility to model non-stationary dynamics. Recent applications in machine learning favor approximate, optimization-based inference for fast predictions, but applications to computer surrogate modeling - with an eye towards downstream tasks like Bayesian optimization and reliability analysis - demand broader uncertainty quantification (UQ). We prioritize UQ through full posterior integration in a Bayesian scheme, hinging on elliptical slice sampling of latent layers. We demonstrate how a DGP's non-stationary flexibility, combined with appropriate UQ, allows for active learning: a virtuous cycle of data acquisition and model updating that departs from traditional space-filling designs and yields more accurate surrogates for fixed simulation effort. We propose new sequential design schemes that rely on optimization of acquisition criteria through evaluation of strategically allocated candidates instead of numerical optimizations, with a motivating application to contour location in an aeronautics simulation. We provide open-source implementations in the "deepgp" package for R on CRAN.

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MS191

Hierarchical Approaches to α-Stable Process Priors

In this talk, we will summarize the recent advancements made for non-Gaussian process priors for statistical inversion. This will be primarily focused on α-stable distributions which provide a natural generalization of a family of distributions, such as the normal and Cauchy. We discuss recently proposed priors which include various Cauchy priors, hierarchical and neural-network based α-stable priors. The focus will be computational where we demonstrate their gains on a range of examples for fully Bayesian and MAP-based estimation. We also provide some theoretical insights which include error bounds.

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MS191

Deep Gaussian Processes and Bayesian Deep Neural Networks

Drawing meaningful conclusions on the way complex real life phenomena work and being able to predict the behavior of systems of interest require developing accurate and highly interpretable mathematical models whose parameters need to be estimated from observations. In modern applications, however, we are often challenged with the lack of such models, and even when these are available they are too computational demanding to be suitable for standard parameter optimization/inference. While probabilistic models based on Deep Gaussian Processes (DGPs) offer attractive tools to tackle these challenges in a principled way and to allow for a sound quantification of uncertainty, carrying out inference for these models poses huge computational challenges which arguably hinder their wide adoption. In this talk, I will present our contributions towards the development of practical and scalable inference for DGPs, which can exploit distributed and GPU computing. In particular, I will discuss how we enable this by relying on the strong connections between DGPs and Bayesian Deep Neural Networks. I will conclude the talk with an overview of recent trends in Bayesian Deep Learning.

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MS191

Computational Methods for Bayesian Imaging with Deep Gaussian Process Priors

In image reconstruction, an accurate quantification of uncertainty is of great importance for informed decision making. Here, the Bayesian approach to inverse problems can be used: the image is represented through a random function that incorporates prior information which is then updated through Bayes' formula. Finding a prior is difficult. Images often exhibit non-stationary effects and multiscale behaviour. Thus, usual Gaussian process priors are not suitable. Deep Gaussian processes, on the other hand, encode non-stationary behaviour in a natural way through their hierarchical structure. To apply Bayes' formula, one commonly employs a Markov chain Monte Carlo method that requires sampling from the prior. In the case of deep Gaussian processes, sampling is especially challenging in high dimensions: the associated covariance matrices are large, dense, and changing from sample to sample. A popular strategy towards decreasing computational complexity is to view Gaussian processes as the solutions to a fractional stochastic partial differential equation (SPDE). In this work, we investigate efficient computational strategies to solve the fractional SPDEs occurring in deep Gaussian process sampling. Indeed, we employ rational approximations to represent the fractional operators through sparse matrices and reduce computational cost from cubic to near-linear. We test our techniques in standard Bayesian image reconstruction problems.

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MS192

Bi-Fidelity Design Under Uncertainty Using Neural Networks

With the ubiquitousness of uncertainty in every engineering system, the robust design of these systems requires addressing the presence of any uncertainty. However, in design under uncertainty, the estimation of response and/or gradients of the response with respect to the design parameters is required for multiple realizations of the uncertainty at every iteration. This may lead to a significant computational cost for the design of large and complex structures. To alleviate this computational burden, in this talk, a computationally efficient bi-fidelity approach is proposed, where a simplified *low-fidelity* model is used along with neural networks to describe the behavior of any nonlinear or design components that represent the complex *high-fidelity* structures behavior together. Once trained, these neural networks provide an inexpensive method to get the structure's response and its gradients with respect to the design parameters for many realizations of the uncertain parameters, reducing the optimization cost. Two numerical examples, namely the design of the base-isolation layer of an 11-story building and the suspension system in a quarter car model, are used to show the efficacy of the proposed approach.

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MS192

Accelerating Bayesian Optimal Experimental Design with Derivative-informed Neural Networks

We consider Bayesian optimal experimental design (BOED) for nonlinear Bayesian inverse problems governed by large-scale partial differential equations (PDEs). For the optimality criteria of BOED, it is common to use expected information gain and some summary statistics, e.g., the trace and determinant of the information matrix that involves the evaluation of the parameter-to-observable map and its Jacobian. However, it is prohibitive to compute these criteria when the PDEs are very expensive to solve, and the parameters to estimate are high-dimensional. To address these challenges, we develop derivative-informed neural network surrogates of the parameter-to-observable map and its Jacobian to accelerate BOED. To tackle the curse-of-dimensionality, we identify and employ suitable dimension reduction techniques to project the parameters and observables into corresponding subspaces. The neural networks are constructed in the subspaces and trained with the Jacobian information in the loss function to significantly enhance the Jacobian approximation accuracy. We demonstrate the efficiency and accuracy of the surrogates in the computation of the parameter-to-observable map, its Jacobian in reduced spaces, the maximum a posteriori (MAP) point, and ultimately the optimality criteria of the BOED compared to high-fidelity finite element approximations. We also show that the proposed method is scalable with respect to the dimensions of the parameters and observables.

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MS193

Diffusion Map Based Langevin Sampler

We propose a Langevin sampler as a generative modelling method. The Langevin sampler is constructed using optimal couplings and diffusion maps. We show how this method can be used to perform inverse modelling tasks as well as providing a stochastic subgrid-scale parametrisation by employing conditional sampling. This is joint work with Sebastian Reich, Fengyi Li and Youssef Marzouk.

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MS193

Data Assimilation in Chaotic Systems Using Reinforcement Learning

Efficient downscaling of large ensembles of coarse-scale information is crucial in several applications, such as climatic modeling. The determining form map is a theoretical lifting function from the low-resolution solution trajectories of an infinite-dimensional dissipative dynamical system to their corresponding fine-scale counterparts. Recently, Hammoud et al. (2022) introduced CDAnet a physics-informed deep neural network as a surrogate of the determining form map for efficient downscaling. CDAnet was demonstrated to efficiently downscale coarse-scale data in a deterministic setting. Herein, the performance of trained CDAnet models is analyzed in a stochastic setting involving observational noise, model noise, and a combination of both noises. The analysis is performed employing the Rayleigh-Benard convection paradigm, under three training conditions, namely, training with perfect, noisy, or downscaled data. The effects of observational and model noise on the downscaled solutions are analyzed. Furthermore, the effects of the Rayleigh number and the spatial and temporal resolutions of the input data on the downscaled fields are examined. The results suggest that the expected L2 error of CDAnet behaves quadratically with the standard deviations of the observational and model noises. The results also suggest that CDAnet responds to uncertainties similar to CDA with an additional error overhead due to CDAnet being a surrogate model.

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MS193

Generative Modelling of Stochastic Parametrisations for Geophysical Fluid Dynamics

We discuss a generative modelling strategy for the stochastic parametrisation of geophysical fluid dynamics models. Stochastic parametrisations are highly desired in fluid dynamics as they enable a principled ensemble generation for forecast and uncertainty quantification applications. Our contribution is a method to learn the stochastic parametrisation as a generative model. We demonstrate the parameterisation as a score-based generative model and discuss the numerical implementation for the rotating shallow-water equations and the simulation results.

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MS193

Ensemble Kalman Methods for Optimization

We consider the ensemble Kalman inversion which has been recently introduced as an efficient, gradient-free optimisation method to estimate unknown parameters in an inverse setting. In the case of large data sets, the ensemble Kalman inversion becomes computationally infeasible as the data misfit needs to be evaluated for each particle in each iteration. Here, randomised algorithms like stochastic gradient descent have been demonstrated to successfully overcome this issue by using only a random subset of the data in each iteration, so-called subsampling techniques. Based on a recent analysis of a continuous-time representation of stochastic gradient methods, we propose, analyse, and apply subsampling-techniques within ensemble Kalman inversion.

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MS194

Gaussian Process Regression on Nested Spaces

As industrial computer codes involve a large amount of input variables, creating directly one big metamodel depending on the whole set of inputs may be a very challenging problem. Industrialists choose instead to proceed sequentially. They build metamodels depending on nested sets of variables (the variables that are set aside are fixed to nominal values). However, at each step, the previous piece of information is lost as a new Design of Experiment is generated to learn the new metamodel. In this paper, an alternative approach will be introduced, based on all the DoEs rather than just the last one. This metamodel uses Gaussian process regression and is called "sequential Gaussian process regression". At each step n, the output is supposed to be the realization of the sum of two independent Gaussian processes Yn-1 + Zn. The first one models the output at step n - 1. It is defined on the input space of step n - 1 which is a subspace of the one of step n. The second Gaussian process is a correction term defined on the input space of step n. It represents the additional information provided by the newly released variables and has the particularity of being null on the subspace where Yn-1 is defined. First, some candidate Gaussian processes for (Zn)n¿2 are suggested, which have the property of being null on an infinite continuous set of points. Then, an EM algorithm is implemented to estimate the parameters of the processes.

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MS194

Hidden But Essential Recipes for Successful Gaussian Process Metamodeling to Support Uncertainty Quantification in Numerical Simulation

The value of using Gaussian Process (GP) regression to emulate costly computational codes for uncertainty management is now widely established. The probabilistic metamodel provided by GP-regression, in the sense that it provides a predictive distribution for each new evaluation point, offers great added value, particularly for safety, reliability or risk assessment studies. However, guaranteeing confidence in the use of this metamodel requires two crucial steps: its training on the available learning data and its validation (often by cross-validation process in our appli-

cation context). We are particularly interested here in the context of given data, small data (number of model simulations limited to a few hundred) and large numbers of uncertain inputs (from a few dozen to a hundred). In this context, building a successful GP metamodel often calls for a preliminary variable selection. Kernel-based methods (HSIC) and associated independence tests are especially appropriate, for screening but also ranking the inputs. Then, particular care is required when estimating GP hyperparameters: going beyond simple maximum likelihood approaches may be wise. Finally, GP validation must include various criteria to assess the preditivity and reliability of the metamodel's entire predictive law. The presentation will focus on recent advances in these three topics, with the aim of providing guidelines and recipes for successful GP metamodeling in the considered application context.

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MS194

Blurring the Distinction Between Data Collection and Computation in Gaussian Processes

The premise of Bayesian modeling is to use posterior uncertainty to represent a quantity of interest that is realized via limited observations. In this talk, I will argue for an analogous notion of *computational uncertainty* when the posterior distribution is realized via limited computation. Focusing on Gaussian process regression, I will introduce an iterative meta-algorithm for posterior inference that returns a combined posterior/computational uncertainty estimate. Just as collecting more data reduces posterior uncertainty, running more iterations of the algorithm reduces computational uncertainty. Extensive experiments demonstrate that accounting for computational uncertainty yields better decision making and generalization. To conclude, I will conclude by discussing how blurring the distinction between data collection and computation can yield new directions for surrogate modeling and decision making.

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MS194

Redefining Model Discrepancy in Calibration: Learning Missing Model Components From Observations

Model discrepancy, formally introduced by Kennedy and OHagan (2001), represents the difference between the physical phenomena and the model output and plays an important role in calibration process. Traditionally, we treat a computer model as a black box and during the calibration process express the observation as the sum of three terms- the simulator output, the model discrepancy and the observation error. However, with the emerging push towards incorporating uncertainty quantification as part of model development where the aim is not only to learn the values of model parameters but also to infer the missing processes from the observations, the current calibration procedure might be insufficient. We propose to redefine the calibration equation and treat the computer model as a grey box, which is a combination of known systems of equations and missing processes of interest that are modelled as Gaussian Processes, effectively bringing the model discrepancy inside the computer model representation. We employ the symbolic regression to replace the outputs of the Gaussian Process with the interpretable mathematical expressions. Due to the probabilistic representation of model discrepancy, we can have a range of mathematical expressions that the modellers can explore and rank. We compare the proposed approach to the principal methods in scientific machine learning and illustrate its performance in an application to Siggaard-Andersen Oxygen Status Algorithm.

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MS195

Grid Total Indices

We consider the estimation of total indices from points arranged on a lattice. We show that these grid total indices are the total indices of a decision-maker who assesses uniform and discrete distributions for the inputs on the grid. We show that making the grid denser and denser, the indices approximate the total indices under any continuous probability measure. We provide several bounds using Poincar-like inequalities and alternative integration techniques. We consider improvements yielded by random shifting or centering the grid.

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MS195

Variable Importance for Random Forests: a Sensitivity Analysis Perspective

Variable importance measures are the main tools to analyze the black-box mechanisms of random forests. Although the mean decrease accuracy (MDA) is widely accepted as the most efficient variable importance measure for random forests, little is known about its statistical prop-

erties. The exact MDA definition varies across the main random forest software. The objective is to analyze the behaviour of the main MDA implementations rigorously, using sensitivity analysis. Consequently, their limits are established when the sample size increases. In particular, these limits are broken down into three components: the first two terms are related to Sobol indices, which are well-defined measures of a covariate contribution to the response variance, as opposed to the third term, whose value increases with dependence within covariates. Thus, it is theoretically demonstrated that the MDA does not target the right quantity when covariates are dependent, which has been noticed experimentally. New important measures for random forests are defined to address this issue: the Sobol-MDA and SHAFF. The Sobol-MDA fixes the flaws of the original MDA and is appropriate for variable selection. On the other hand, SHAFF is a fast and accurate estimate of Shapley's effects, even when input variables are dependent. SHAFF is appropriate to rank all variables for interpretation purposes. The consistency of the Sobol-MDA and SHAFF is proved, showing that they empirically outperform their competitors.

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MS195

Unveiling the Path to Desired Predictions: An Interpretability Approach for Black-Box Models

As machine learning models continue to be widely adopted in various deployed decision systems, their inherently nature as black-box models underscores the increasing necessity for explaining their predictions. While popular explainable machine learning methods proficiently furnish insights into the most influential features of individual predictions, they fall short in providing guidance to agents seeking to transition between different prediction classes. This work introduces an approach grounded in finite change decomposition and Shapley values, designed to uncover actionable insights concerning the desired trajectory of predictions. Through the application of this method across multiple UCI datasets, a diverse range of technical and managerial insights is presented.

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MS195

Modified Pick-and-Freeze Design for Total Effects with Constrained Features

Total effects are variance-based sensitivity measures which report the difference between the variance of the model output and the portion of the output that remains after all features have been fixed, with the exception of the feature of interest. For their computation, pick-and-freeze designs together with Jansen's variance estimation are frequently used. Even in the case of dependent features, total effects retain an interpretation from a relative error perspective. However, the presence of statistical dependence prevents a straight-forward computational treatment. We present a method to augment the pick-and-freeze design with weight factors to compensate for the dependence or constraints in the features. We show asymptotic properties of this estimator, drawing upon results from U-statistics theory. We also test nearest neighbor methods to obtain a data-driven estimate for total effects.

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MS197

A Scalable Bayesian Framework for Spatiotemporal Imaging Spectroscopy

Data assimilation for spatiotemporal analysis is often framed as the extension of spatial modeling to the temporal domain. Traditionally, methods have centered on scalar fields due to the high dimensionality of the spatial domain. However, many real-world scenarios involve a collection of correlated quantities of interest, prompting the challenge of modeling multivariate fields over both spatial and temporal domains. We present a Bayesian spatiotemporal modeling framework, based on transportation of measure, that extends to multivariate quantities of interest and can in principle handle non-Gaussianity. We highlight specific application to the problem of imaging spectroscopy retrievals in Earth remote sensing.

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MS197

Multilevel Delayed Acceptance MCMC

We develop a novel Markov chain Monte Carlo (MCMC) method that exploits a hierarchy of models of increasing complexity to efficiently generate samples from an un-normalized target distribution. Broadly, the method rewrites the multilevel MCMC approach of Dodwell et al [SIAM/ASA J Uncertain Quantif, 3, 2015] in terms of the delayed acceptance MCMC of Christen and Fox [J Comput Graph Statist, 14, 2005]. In particular, delayed acceptance is extended to use a hierarchy of models of arbitrary depth and allow subchains of arbitrary length. Weshow that the algorithm satisfies detailed balance and hence is ergodic for the target distribution. Furthermore, multilevel variance reduction is derived that exploits the multiple levels and subchains, and an adaptive multilevel correction to coarse-level biases is developed. Three numerical examples of Bayesian inverse problems are presented that demonstrate the advantages of these novel methods. The software and examples are available in PyMC3

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MS197

Semi-Autoregressive Energy Flows in High Dimensions

Normalizing flows have typically been used to represent likelihood-based representations of high-dimensional data distributions by mapping complex distributions to simple distributions through invertible transformations. Their advantages in modeling high dimensional invertible data contributes to their applicability to Bayesian inversion problems. However, training normalizing flow generative models can be challenging due to the need to calculate computationally expensive determinants of Jacobians, and typically require restricted architectures to make the inversion stable and efficient at training time. We apply the energy objective, an alternative sample-based loss based on proper scoring rules, in order to make a normalizing flow model determinant-free in training while supporting flexible model architectures that are not easily compatible with maximum likelihood training. These properties allow us to introduce a novel model family of flows called semi-autoregressive energy flows that interpolates between fully autoregressive and non-autoregressive models.

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MS197

Tensor-Train Methods for Sequential State and Parameter Estimation in State-Space Models

Numerous real-world applications require the estimation, forecasting, and control of dynamic systems using incomplete and indirect observations. These problems can be formulated as state-space models, where the primary challenge lies in learning the models states and parameters from observed data. In this talk, we will present new tensor-train-based sequential learning methods that jointly estimate parameters and states under the Bayesian framework. Our methods, viewed from the function approximation perspective, provide manageable error analysis and potentially mitigate the particle degeneracy encountered in many particle-based approaches. Besides offering new insights into algorithmic design, our methods naturally incorporate conditional Knothe–Rosenblatt rearrangements, enabling filtering, smoothing, and parameter estimation within a unified framework. We will also discuss several preconditioning techniques to improve the efficiency of our methods. Tested on several state-space models, including the Kalman filter, the stochastic volatility model, and the predator-prey model, our methods deliver state-of-the-art accuracy and computational performance.

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MS198

An Alternative Approach to Standard Methods of Covariance Propagation

The propagation of the error covariance is an important aspect of the statistical estimation of dynamical systems, such as data assimilation. Two major problems arise with standard methods of covariance propagation: spurious loss of variance, in which the estimated variance underapproximates the exact variance, and computational expense, as the explicit propagation of the covariance matrix is computationally intense, even in modest sized systems. In this presentation, we introduce an alternative approach to covariance propagation that can mitigate both these issues. Rather than evolving the full covariance or approximating it a low rank, we evolve the variance field and correlation length field, then reconstruct the covariance using a parametric correlation function. For example, the variance and correlation length fields for advective dynamics are each governed by a partial differential equation (PDE) in N dimensions, where N is the number of space dimensions of the state. Thus, we can approximate the full covariance without solving the covariance PDE, which is in $2N$ space dimensions, by solving just two PDEs each in only N space dimensions. This approach can reduce computational costs relative to standard methods of covariance propagation and mitigates spurious loss of variance by evolving the variance directly. We conclude this presentation with preliminary results for one-dimensional advective dynamics and briefly discuss its extension to higher dimensions.

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MS198

Data-Driven Learning for Mori-Zwanzig Formalism: Theory and Potential Applications

More than half a century ago, Mori and Zwanzig (MZ) developed a mathematically rigorous formalism for constructing reduced-order models for dynamical systems using functional projection operators. Several recent studies have established that with Mori's linear projection operator, it is possible to adopt a data-driven approach to learn the MZ operators using the time series of the resolved dynamics. In this talk, I will present our latest proposition of using regression analysis to define the projection operators, and a data-driven method for learning the associated MZ operators using time-series data. The newly proposed method can be considered as a generalization of our recently proposed method (Lin et al. 2021, SIADS) because it is not restricted to linear regressions. As we gradationally increased the complexity of the regression models, we observed a consistent improvement of the learned reduced-order models on a few test examples. We still observed considerable improvements by including the MZ memory effect in these nonlinear projections, justifying the necessity of accounting for the past histories of under-resolved systems. We believe that the proposed method for learning MZ operators is promising because it is applicable to most data-driven methods (e.g., approximate Koopman and SINDy) for learning dynamical systems.

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MS198

Stochastic Closures for Real-time Fluid Applications

We are interested in real-time estimation of 3D fluid flows, using limited computational resources. This is possible through the coupling between synthetic data, physical models and sparse fluid flow measurements. Combining synthetic data and models, intrusive Reduced Order Model (ROM) drastically reduce the problem dimensionality. Unfortunately, even with corrections, the accumulated errors of these surrogate models increase rapidly over time. Stochastic closures (SC) and Data assimilation (DA) can alleviate these problems. SC provide a set of simulations covering probable futures (Uncertainty Quantification problem) and DA constraints these online simulations with measurements. Our SC is a multi-scale physics-based Markovian model with correlated additive and multiplicative noises, calibrated with new statistical estimators [Resseguier et al. (2021). SIAM-ASA J. Uncertain. Quantif., 9(3), 1152-1183]. Then – from a particle filter assimilating measurements at a single location in space – our method greatly exceeds the state of the art, for ROM degrees of freedom smaller than 10 and moderately turbulent 3D flows [Resseguier et al. (2022). J. Comput. Phys., 471, 111631]. Recently, we have obtained similar results with our new implementation in the finite-volume code OpenFOAM and the ROM library ITHACA-FV [Stabile Rozza (2018). Comput. Fluids., 173:273284]. We are now addressing turbulent flows, with Large Eddy Simulation (LES), hyperreduction and new dedicated SC.

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MS199

Case Studies for Statistical Finite Element Methods in Shallow Water

In this talk I will present the statistical finite element method and demonstrate it's effectiveness on various case studies in shallow water. This *statFEM* is a novel augmentation of the classical finite element method which admits misspecification in the governing equations in order to update their solutions, *a posteriori*, with data. The resultant posterior distribution characterises all sources of uncertainty in the governing system, given model assumptions, hyperparameters, and data. In application, shallow water is perhaps the most common setting of large-scale fluid-flow on the planet and presents an investigation of utmost importance. We will present results with synthetic and experimental data, demonstrating that the method is able to provide a statistically coherent synthesis of models and data, which is able to correct for model misspecification via potentially sparse observation systems. Joint work with Edward Cripps, Thomas Stemler, Paul Branson, Matt Rayson, and Mark Girolami.

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MS199

Physics-Informed Dynamical Vaes for Unstructured Data Assimilation

Incorporating unstructured data into physical models is a challenging problem that is emerging in data assimilation. Traditional approaches focus on well-defined observation operators whose functional forms are typically assumed to be known. This prevents these methods from achieving a consistent model-data synthesis in configurations where the mapping from data-space to model-space is unknown. To address these shortcomings, we develop a physics-informed dynamical variational autoencoder (ϕ-DVAE) to embed diverse data streams into time-evolving physical systems described by differential equations. A variational Bayesian framework is used for the joint estimation of the encoding, latent states, and unknown system parameters. Unstructured data, in our example systems, comes in the form of video data and velocity field measurements. To demonstrate the method, we provide case studies with the Lorenz-63 ordinary differential equation, and the advection and Korteweg-de Vries partial differential equations. Our results, with synthetic data, show that F-DVAE provides a data efficient dynamics encoding methodology which is competitive with standard approaches. Unknown parameters are recovered with uncertainty quantification, and unseen data are accurately predicted.

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MS199

Learning Aerosol Dispersion with Langevin Surrogate Dynamics

For decades, satellite imagery has been able to detect ship tracks, temporary cloud trails created via emitted aerosol injections from ships. These are satellite-observable examples of aerosol-cloud interactions, dynamic processes that constitute the largest uncertainty in climate forcing predictions. Further, they highlight the ability of aerosols in altering the albedo of the atmosphere and contributing to indirect radiative forcing. To quantify the potential of aerosol injections on the surrounding climate, high-resolution Large Eddy Simulations (LES) can be used to capture the changing dynamics of aerosol injections. However, due to large computational constraints and the challenges in LES comparison with satellite imagery, reduced-order models are required for improved assessments. In this talk, we illustrate a novel stochastic Langevin representation of injected aerosol trajectories, that importantly accounts for dispersion-driving turbulence parameters and variable wind fields. Under this model, we show accurate comparisons with LES under a variety of atmospheric and cloud conditions, by matching spreading rates of the resulting tracks. Finally, we use this parameterization to analyze real ship tracks observed from satellite under both slow and fast spreading case-studies.

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MS200

Openturns: Features and Graphical Interface

OpenTURNS is an open source C++ library for uncertainty propagation by probabilistic methods. Developed in a partnership of five companies and institutions (EDF, Airbus, ONERA, Phimeca and IMACS), it benefits from constant user feedback. Classical algorithms of UQ (central dispersion, probability of exceedance, sensitivity analysis, metamodels) are available and efficientely implemented. Connecting a new simulator to OpenTURNS is easy, thanks to various wrapper services. The OpenTURNS Python module, built on top of the C++ library, is the interface that most users commonly know in practice. However there are situations where we want to perform a UQ study without using a programming language. This is why we developped Persalys, a graphical user interface (GUI) of OpenTURNS, with the goal of increasing the use of OpenTURNS and, more generally, of the UQ methodology. Through examples, we discuss the main features of the tool: central dispersion analysis, global sensitivity analysis and threshold probability estimate. We also present advanced graphical features, including the interactive plot matrix view and the parallel coordinate plot available in the GUI and based on the Paraview framework. Finally, we show how the interface can be used within a HPC context, with only limited input from the user.

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MS201

Sampling with Approximate Transport Maps

Deep generative models parametrize very flexible families of distributions able tofit complicated datasets of images or text. These models provide independent samples fromcomplex high-distributions at negligible costs. On the other hand, sampling exactly a targetdistribution, such a Bayesian posterior or the Boltzmann distribution of a physical system, is typically challenging: either because of dimensionality, multi-modality, ill-conditioning or a combination of the previous. In this talk, I will discusshow

to enhance traditional inference and sampling algorithms with generative models based on transport maps.

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MS201

Clustering in Transformers: An Interacting Particle Systems Perspective

This talk will report on several results, insights and perspectives Cyril Letrouit, Yury Polyanskiy, Philippe Rigollet and I have found regarding Transformers. We model Transformers as interacting particle systems (each particle representing a token), with a non-linear coupling called self-attention. When considering pure self-attention Transformers, we show that trained representations cluster in long time to different geometric configurations determined by spectral properties of the model weights. We also cover Transformers with layer-normalisation, which amounts to considering the interacting particle system on the sphere. On high-dimensional spheres, we prove that all randomly initialized particles converge to a single cluster. The result is made more precise by describing the precise phase transition between the clustering and non-clustering regimes. The appearance of metastability, and ideas for the low-dimensional regime, will be discussed.

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MS201

Diffeomorphic Measure Matching with Kernels for Generative Modeling

We present a general framework for the transport of probability measures towards minimum divergence generative modeling and sampling using ordinary differential equations (ODEs) and Reproducing Kernel Hilbert Spaces (RKHSs), inspired by ideas from diffeomorphic matching and image registration. A theoretical analysis of the proposed method is shown, giving a priori error bounds in terms of the complexity of the model, the number of samples in the training set, and model misspecification. An extensive suite of numerical experiments further highlights the properties, strengths, and weaknesses of the method and extends its applicability to other tasks, such as conditional simulation and inference.

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MS201

A Generative Flow for Conditional Sampling via Optimal Transport

Sampling conditional distributions is a fundamental task for Bayesian inference and density estimation. Generative models, such as normalizing flows and generative adversarial networks, characterize conditional distributions by learning a transport map that pushes forward a simple reference to a target distribution. While these approaches successfully describe many non-Gaussian problems, their performance is often limited by parametric bias and the reliability of gradient-based (adversarial) optimizers to learn these transformations. This work proposes a non-parametric generative model that iteratively maps reference samples to the target. The model uses block-triangular transport maps, whose components are shown to characterize conditionals of the target distribution.

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MS202

Ergodicity of a Stochastic Quasi-Geostrophic Model via Generalised Coupling Method

A two-layer quasi-geostrophic model for geophysical flows is studied, with the upper layer being perturbed by additive noise. This model is popular in the geosciences, for instance to study the effects of a stochastic wind forcing on the ocean. A rigorous mathematical analysis however meets with the challenge that in the model under study, the noise configuration is spatially degenerate as the stochastic forcing acts only on the top layer. In this talk we give an overview of results on ergodic properties of this model. The approach used provides a general framework for generalised coupling techniques suitable for applications to dissipative SPDEs.

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MS202

Geometric Deep Neural Operators for Bayesian Inverse Problems

Bayesian inverse problems (BIPs) are often prohibitive to

solve when the parameters represent discretized infinite dimensional fields and when the forward problem is governed by expensive-to-solve PDEs. Efficient evaluation of the map from parameters to observables, which involves solution of the forward PDEs, is key to making the solution of BIPs tractable. Efficient surrogate approximations of these maps can greatly accelerate solution of BIPs, provided an accurate surrogate can be trained with modest numbers of PDE solves. Unfortunately, constructing such surrogates presents significant challenges when the discretized parameter dimension is high and the forward model is expensive. Neural operators have emerged as leading contenders for overcoming these challenges. We demonstrate that black box application of neural operators leads to poor results when training data are limited due to the expense of the forward PDEs. Instead, by constructing a network architecture that captures the geometry of the map—its smoothness, anisotropy, and intrinsic low-dimensionality—as revealed through adjoint-based Gauss-Newton Hessians, one can construct a dimension-independent reduced basis geometric neural operator with superior generalization properties using just limited training data. We employ this neural operator to make tractable the solution of PDE-constrained BIPs.

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MS202

Application of Information Geometry in Uncertainty Quantification: Insight and Challenges

Mathematical models play a crucial role in scientific exploration, helping us to encapsulate our understanding of complex physical systems and tackle domains that are experimentally challenging or impossible. Uncertainty quantification (UQ) serves as a vital tool for evaluating a model's reliability. However, many multi-parameter models, spanning various disciplines, exhibit a phenomenon known as "sloppiness," wherein they are largely insensitive to coordinated changes in multiple parameter combinations. This can result in confidence regions within a model's parameter space that do not close, effectively allowing an infinite range of physically plausible parameter values. Within the context of Markov Chain Monte Carlo (MCMC) sampling for Bayesian posterior analysis, this sloppiness phenomenon leads to "parameter evaporation," where samples tend to favor sub-optimal regions at some sampling temperatures. In this study, we delve into this phenomenon and leverage information geometry to illuminate the impact of model sloppiness on traditional uncertainty quantification methods, such as MCMC. While our investigation primarily centers on models of interatomic potential used in materials science, the insights presented extend to models in various fields. This research sheds light on the broader implications of sloppiness and enhances our understanding of uncertainty in mathematical models.

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MS202

Using Data-Consistent Inversion to Build Population-Informed Priors for Bayesian Inference

Conditioning prior estimates of uncertainty on observational data, via Bayesian inference, is essential when building predictive digital twins of physical assets. However, it is difficult to substantially reduce uncertainty in digital twin predictions when solely utilizing data from a single individual asset. Consequently, we propose utilizing data from a population of related assets to construct informative priors that can be used to reduce uncertainty in the digital twin of any single asset. Specifically, we use data consistent inversion, which given an uninformative prior, forms an informative prior that when pushed forward through the observation operator matches the observed probability density of the population data. Our numerical examples demonstrate that utilizing population-informed priors significantly increases the KullbackLeibler divergence from the posterior to the prior in comparison to utilizing uninformative priors. These results are complemented with theory for linear-Gaussian inference that establishes the conditions under which using our approach is guaranteed to improve posterior estimates of uncertainty.

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MS203

Efficient Inference and Identifiability Analysis for Models with Random Parameters

Heterogeneity is a dominant factor in the behaviour of many biological processes and is often a significant source of the variation observed in biological data. Despite this, it is relatively rare for mathematical models of biological systems to incorporate variability in model parameters as a source of noise. In this talk, we develop a computationally efficient method for inference and identifiability analysis of so-called random parameter models based on an approximate moment-matched solution constructed through a multivariate Taylor expansion. Overall, we show how analysis of random parameter models can provide more precise parameter estimates and more accurate predictions with minimal additional computational cost compared to traditional modelling approaches. Importantly, our method is highly transferrable and easily applicable to a broad class of deterministic models.

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MS203

Multimodel Inference to Account for Model Uncertainty in Systems Biology

When modeling biological systems, it is often possible to formulate a set of related mathematical models that vary in the simplifying assumptions used to represent the system mathematically. One should account for the uncertainties associated with these assumptions when making predictions. Model selection and discrepancy modeling allow one to choose the best model and account for model uncertainty by considering the mismatch between data and predictions. However, given the limited data in systems biology, these approaches may lead to biases and misrepresentations of uncertainty due to selecting a single model. In this talk, we highlight several methods for multimodel inference that leverage the entire set of models to avoid selection biases and account for model uncertainty by incorporating contributions from all models. Methods including pseudo-Bayesian model averaging, stacking of predictive densities, and probability density fusion, construct robust predictors using the entire model family and avoid conditioning predictions on one model. We highlight multimodel inference with examples of mitogen-activated protein kinase (MAPK) signaling, a system responsible for regulating cell growth and implicated in many cancers. Our results show how multimodel inference accounts for model uncertainty and, thus, improves predictive certainty and reduces model selection bias.

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MS203

InVAErt Networks: a Data-Driven Framework for Model Synthesis and Identifiability Analysis

Use of generative models and deep learning for physics-based systems is currently dominated by the task of emulation. However, the remarkable flexibility offered by data-driven architectures would suggest to extend this representation to other aspects of system synthesis including model inversion and identifiability. We introduce inVAErt (pronounced *invert*) networks, a comprehensive framework for data-driven analysis and synthesis of parametric physical systems which uses a deterministic encoder and decoder to represent the forward and inverse solution maps, a normalizing flow to capture the probabilistic distribution of system outputs, and a variational encoder designed to learn a compact latent representation for the lack of bijectivity between inputs and outputs. We formally investigate the selection of penalty coefficients in the loss function and strategies for latent space sampling, since we find that these significantly affect both training and testing performance. We validate our framework through extensive numerical examples, including simple linear, nonlinear, and periodic maps, dynamical systems, and spatio-temporal PDEs.

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MS203

Improving Multifidelity Uncertainty Propagation for Cardiovascular Applications Through Dimensionality Reduction Techniques

We consider the problem of estimating expectations of quantities of interest of computationally expensive models, such as cardiovascular simulations, when the distribution of the random inputs is either known analytically or provided through samples. We assume that a cheaper low-fidelity surrogate of the high-fidelity model is available, and we develop novel multifidelity estimators with the twofold purpose of increasing the range of applicability and reducing the variance of the standard multifidelity Monte Carlo estimator. In particular, we allow the high-fidelity and low-

fidelity models to have dissimilar parameterizations, meaning that the number of random inputs or their distribution can be different. This is a common situation in cardiovascular applications, where the surrogate model can be a substantial simplification of the 3D model. We achieve this generalization by building a shared subspace of reduced dimension through normalizing flows and either linear or nonlinear dimensionality reduction techniques, i.e., active subspaces and autoencoders, respectively. These transformations capture the direction of maximum change of the high-fidelity and low-fidelity models, and consequently they lead to an increased correlation between the models, which in turn yields estimators with reduced variance. We show the advantages of our approaches through several numerical experiments.

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MS204

Reconstructing Joint Densities from Marginals by Time-Delay Embedding

We discuss how to transport marginal densities obtained through projection from a joint, but assumed unknown, density, into a more informative, higher-dimensional joint space. To construct the higher-dimensional space, we mainly leverage time-delayed measurements from an observation process. Our approach can augment the information from scientific equipment to construct a more coherent view. In numerical experiments, we reconstruct the surface of an implant from partial recordings of bacteria moving on it, and construct a joint space for satellites orbiting the Earth by combining one-dimensional, time-delayed altitude measurements.

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MS204

Approximative Likelihoods for Chaotic and Stochastic Dynamical Systems

A generic way to construct likelihoods for both chaotic and stochastic differential equations is presented. The method provides a model-agnostic estimation procedure for situations often described as intractable. For 'small' data sets the approach is combined with the Bayesian synthetic likelihood approach, while situations with 'large' data sets and high CPU demands are dealt with by dividing the data in subsets. The examples on chaotic systems are motivated by weather prediction models, where stochasticity is introduced by randomizing the model parameters and dynamics in a highly nonlinear way. Both basic test cases and analysis of the operational-scale weather model OpenIFS are discussed.

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MS204

Active Learning of Energy Based Models Using Stochastic Stein Variational Gradient Descent

Energy-based models provide a unified framework for approximating complex target distributions in machine learning, but typically require abundant labeled data to fit. Active learning aims to make model fitting more efficient by iteratively and adaptively constructing informative training datasets. This work proposes a sampling-based approach for the active learning of energy-based models, in a setting where labels for new training samples may be accessed via an oracle, such as an expensive simulation model. We introduce an algorithm which alternates between sampling from the invariant distribution of an energy-based model using a variant of stochastic Stein variational gradient descent and updating the energy-based model by maximum likelihood estimation using the augmented training set. The trajectory interacts with existing training samples to promote diversity in newly sampled data, but retains fidelity to the target distribution under appropriate assumptions. We develop criteria for querying the oracle in an iterative active learning scheme, derive asymptotic properties of the algorithm, and demonstrate its efficiency in the context of surrogate model construction and generative modeling.

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MS205

Efficient Geometric MCMC for PDE-Constrained Bayesian Inversion Enabled by Derivative Informed Neural Operator

This talk presents an operator learning approach to accelerate PDE-constrained Bayesian inversion. This ap-

proach involves building a surrogate of the parameter-to-observable map and its parametric derivative, or Jacobian, via training a derivative-informed neural operator (DINO). The learned operator is then used to efficiently generate proposals for function space geometric MCMC. DINO is a model reduction neural operator trained via approximation error minimization in the topology of the H^1 Sobolev space with a Gaussian measure. DINO leads to meaningful Jacobian evaluations for high-dimensional input. When used to generate MCMC proposals for Bayesian inversion, DINO allows rapid sampling from local Gaussian approximations of posterior distributions and fast estimations of the acceptance ratio. We demonstrate that our proposed MCMC procedure based on DINO employs a nonlinear dimension reduction of the parameters space via parametrically rotating the pre-determined reduced basis. Preliminary numerical examples that test the efficiency of the proposed approach are provided.

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MS205

Certifiable Low-Dimensional Structure in Bayesian Inference Using Dimensional Logarithmic Sobolev and Poincare Inequalities

Inference in the Bayesian paradigm is completely characterized by the posterior distribution. However, accessing this high-dimensional probability measure poses significant computational challenges. To that end, we construct low-dimensional approximations to this distribution using a gradient-based algorithm derived from Markov semigroup inequalities. Our resulting approximation is furnished with certifiable and computable error guarantees. Of note, we identify linear low-dimensional subspaces which exert universal control over the 'worst-case' approximation error with respect to the Amari alpha-divergences. By leveraging recent advances in the study of functional inequalities, namely the dimensional logarithmic Sobolev and Poincaré inequalities, we also obtain refined subspaces which result in an order of magnitude improvement in error guarantees for the KL divergence and squared Hellinger metric, respectively.

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MS205

Derivative-informed Deep Operator Network

Deep operator networks, a class of neural operators that learn mappings between function spaces, have recently been developed as surrogate models for parametric partial differential equations (PDEs). In this talk, we introduce a derivative-informed deep operator network (DI-DeepONet), which leverages the derivative information of the solution operator of parametric PDEs to enhance the accuracy and efficiency of DeepONet. DI-DeepONet uses DeepONet as its backbone and incorporates two derivatives in the loss function for training, including the directional derivatives of the output function with respect to the input function and the gradient of the output function with respect to the physical domain variables. This feature enhances generalization accuracy, especially in scenarios with limited training data, and provides a more accurate approximation of derivatives. Additionally, we propose to use a reduced representation of the input functions (e.g., through projection into the KarhunenLove expansion subspace or the active subspace) rather than the full representation. The model-based dimension reduction of input functions allows us to train a much smaller neural network, thereby significantly reducing the computational cost for training and the required volume of training data. We present the results of several numerical experiments to demonstrate the effectiveness of DI-DeepONet compared to DeepONet.

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MS206

Autocalibration of the E3SM Version 2 Atmosphere Model Using a PCA-Based Surrogate for Spatial Fields

Global Climate Model (GCM) tuning (calibration) is a time-consuming process, with high-dimensional input and output fields. Experts typically tune by iteratively running climate simulations with hand-picked values of tuning parameters. Many, in both the statistical and climate literature, have proposed alternative calibration methods, but most are difficult to implement. We present a practical, robust, and rigorous calibration approach on the atmosphere-only model of the Department of Energys Energy Exascale Earth System Model (E3SM) version 2. Our approach can be summarized into two parts: (1) the training of a surrogate, and (2) gradient-based parameter optimization. To train the surrogate, we generate a set of designed ensemble runs that span our input parameter space and use polynomial chaos expansions on a reduced output space to fit the E3SM output. We use this surrogate in an optimization scheme to identify values of the input parameters for which our model best matches gridded spatial fields of climate observations. To validate our choice of parameters, we run E3SMv2 with the optimal parameter values and compare prediction results to expertly-tuned simulations

across 45 different output fields. This flexible, robust, and automated approach is straightforward to implement, and we demonstrate that the resulting model output matches present day climate observations as well or better than the corresponding output from expert tuned parameter values.

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MS206

Surrogate-Accelerated Parameter Optimization for the Quasi-Biennial Oscillation

The quasi-biennial oscillation (QBO) is the leading mode of climate variability in the tropical stratosphere characterized by alternating patterns of westerly and easterly winds. Though it is confined to the equatorial region, it influences weather and climate patterns globally via teleconnections. Of particular interest is the zonal wind amplitude over time within the westerly and easterly regimes. We develop and implement an efficient uncertainty quantification workflow to optimize physics parameters and calibrate the representation of the resolved and parameterized gravity waves in the Energy Exascale Earth System Model. We create a compact representation of the QBO amplitude over multiple pressure levels by coupling a Karhunen-Love based dimensionality reduction and a polynomial chaos expansion to efficiently simulate the amplitude at a fraction of cost while also extracting sensitivity indices to rank the physical parameters according to their impact on the oscillation amplitude. Additionally, we carry out a surrogate-accelerated calibration via Bayesian inference using the atmospheric reanalysis data as a reference metric to find a set of parameter values producing a more realistic QBO.

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MS206

From Earth System Models to Decisions: The Roles of Variability, Uncertainty, and Predictabil-

may benefit from physics-informed machine learning, with uncertainties resulting from imperfect physics and data-driven models. At subseasonal to interannual scales, multimodel superensembles attempt to account for uncertainties in initial conditions and model physics with multiple numerical weather prediction models and many initial states. At decadal to century scales, climate projections rely on simulations from earth system model ensembles, where forcings and model spread represent knowledge gaps in human and natural systems, and initial condition runs represent internal variability. The variability in simulations translates to uncertainty in projections. Uncertainties may be magnified if data-driven methods are used to generate projections at stakeholder-scales. This presentation discusses these challenges with an emphasis on uncertainty quantification, and discusses how solutions may be developed by taking into account methods drawn from information theory, nonlinear physics, and statistics. Case studies include precipitation nowcasting for water resources engineering and regional climate assessments for hydrologic science.

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MS206

Uncertainty Quantification of Atmospheric Transport Modeling of Fallout from Historic Nuclear Tests

Manhattan Project scientists were wary in the days and hours leading up to the Trinity test due to many physics and engineering uncertainties. They were also anxious about whether radioactive fallout from Trinity would impact downwind populated areas sixty or more kilometers away. Uncertainty in meteorology, multi-modal fallout distributions, and mushroom cloud geometry can all affect the transport, dispersion, and deposition of fallout in the atmosphere. Quantifying fallout uncertainty may also improve the ability to simulate other closely related phenomena in earth system models, including the transport of smoke and ash plumes from wildfires and volcanic eruptions. To better understand fallout and related climate processes, we applied uncertainty quantification to atmospheric simulations and measurements of historic above-ground nuclear tests. Monte Carlo simulations of fallout are used to train data-driven algorithms for quick forward and inverse probabilistic analyses. In the forward direction, the algorithms provide probability distribution functions of spatial fallout patterns, given inputs related to the device, environment,

with a small number of summary-level measurements.

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MS207

Information Bottleneck Based Uncertainty Quantification for Scientific Machine Learning

In this talk, we will present a novel framework for uncertainty quantification via information bottle- neck (IB-UQ) for scientific machine learning tasks, including deep neural network (DNN) regression and neural operator learning (DeepONet). In comparison to uncertainty quantification (UQ) methods for scientific learning tasks that rely on Bayesian neural networks with Hamiltonian Monte Carlo posterior estimators, the model we propose is computationally efficient, particularly when dealing with large-scale data sets. The effectiveness of the IB-UQ model is demonstrated through several representative examples.

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MS207

Assessments of Epistemic Uncertainty Using Gaussian Stochastic Weight Averaging for Fluid-flow Regression

We use Gaussian stochastic weight averaging (SWAG) to assess the epistemic uncertainty associated with neural-network-based function approximation relevant to fluid flows. SWAG approximates a posterior Gaussian distribution of each weight, given training data, and a constant learning rate. Having access to this distribution, it is able to create multiple models with various combinations of sampled weights, which can be used to obtain ensemble predictions with quantified model-form uncertainty. This approach is applied and evaluated for uncertainty quantification of various inverse problems in computational fluid dynamics.

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MS207

Quantifying Uncertainties in Weight-Parameterized Residual Neural Networks

Neural network (NN) have been employed as surrogates to replicate input-output maps in complex physical models, accelerating sample-intensive studies such as model calibration and sensitivity analysis, albeit in most instances trained NNs are treated deterministically. In the context of probabilistic estimation, Bayesian methods provide an ideal path to infer NN weights while incorporating various sources of uncertainty in a consistent fashion. However, exact Bayesian posterior distributions are extremely difficult to compute or sample from. Variational approaches, as well as ensembling methods, provide viable alternatives accepting various degrees of approximation and empiricism. This work focuses on special NN architectures, residual NNs (ResNets). Inspired by the continuous, neural ODE analogy, we develop an approach for ResNet weight matrix parameterization as a function of depth. The choice of parameterization affects the capacity of the network, leading to regularization and improved generalization. More importantly, weight-parameterized ResNets become more amenable to Bayesian treatment due to the reduction of the number of parameters and overall regularization of the loss, or log-posterior, surface. We will highlight the improvements in training and generalization gained by using weight-parameterized ResNet architectures in the context of various Bayesian NN learning methods.

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MS208

Overcoming Fear of Missing Out (FOMO): Active Selection of Training Data to Predict Extreme Event Statistics in Climate Datasets

As the severity and frequency of extreme weather events increases, the ability to predict these is becoming both more important and more difficult. The broad range of dynamically relevant spatiotemporal scales in the Earths atmosphere makes direct numerical simulations computationally expensive and simplified data-driven approaches inaccurate. Scientific machine learning methods are a useful substitute but are slow or intractable for large datasets. We introduce an active learning framework that identifies data points most relevant to the dynamics of extreme weather events. Our framework uses an output-weighted sampling criterion to sequentially select optimal training input points that give rise to outputs in the tails of the distribution (i.e. extreme events). To compute the criterion, we quantify the uncertainty in our model using neural network architectures capable of making probabilistic predictions. We test our method on a dispersive nonlinear wave model and on the ERA5 climate dataset. In both cases, we find that the machine learning models achieve the highest accuracy with the fewest number of points when trained on data selected by our output-weighted search algorithm. Lastly, we use clustering to interpret the physical meaning

of the optimally selected points.

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MS208

Extremes of Switching Diffusion Models

High-fidelity simulations, crucial for elucidating rare phenomena such as failure and system instabilities, often pose insurmountable computational challenges that impede systematic statistical analysis of these events. This research addresses this limitation by developing an innovative probabilistic framework called the hybrid switching diffusion model (HSD), to uncover and quantify rare events in simulations, with a particular focus on linking micro-scale features to macro-scale behaviors. Utilizing a switching diffusion model, we efficiently generate sample paths with prescribed statistical properties, allowing for the rigorous examination of rare event probabilities, a capability that surpasses traditional multi-variate extreme value theory. This approach yields an advancement in the study of rare events within high-fidelity simulations, enhancing our capacity to understand, predict, and mitigate such occurrences in critical applications like material analysis and fluid dynamics.

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MS208

Efficient Conditional Sampling of Max-Stable Processes

Max-stable processes arise from an infinite-dimensional generalization of extreme value theory, and are the natural class of processes to consider when sample maxima are observed at each site of a spatial process. We propose new algorithms for efficient conditional sampling of max-stable processes, which are useful in exploring and using the dependence among extremes. Given a max-stable process $M(x)$, we consider its spectral decomposition with Gumbel marginals, $M(x) = \max_{n\geq 1} J_n(x) - \log A_n$, where J_n are i.i.d samples from a sub-Gaussian spectral density and A_n is the n-th arrival of a Poisson process independent of each J_n. Our initial approach assumes a multivariate normal spectral density with non-diagonal covariance and truncates the maximum over a finite number of samples N. We use a triangular transformation to expose the dependence among components of each J_n, and then formulate conditional sampling as sequential sampling of *a priori* independent random variables subject to a system of linear constraints, which we perform by studying the sequential likelihood ratios. We discuss the efficiency of this procedure and its extensions.

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MS208

Fracture Statistics in Polymer Networks: A Branching Random Walk Analysis

Recent studies established a connection between the macroscopic mechanical response of polymeric systems and the statistics of the shortest path (SP) length between distant cross-links. Since these statistics can be costly to compute and difficult to study theoretically even in computational models (let alone in real systems), we introduce a branching random walk (BRW) model to represent the polymer network morphology in coarse-grained molecular dynamics (CGMD) simulations. We postulate that the first passage time (FPT) of the BRW to a given termination site can be used to approximate statistics of the SP between distant cross-links in the polymer network. We develop a theoretical framework for studying the FPT of spatial branching processes. In particular, our results yield an analytical expression for estimating the FPT distribution as a function of the cross-link density. We demonstrate by extensive numerical calculations that the distribution of the FPT agrees well with the SP distribution from the CGMD simulation. The theoretical estimate and the subsequent numerical scheme provide an efficient way of approximating the SP distribution in a polymer network. Our work presents the first analysis of polymer networks as a BRW and sets the framework for developing a generalizable spatial branching model for studying the macroscopic evolution of polymeric systems.

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MS209

Pareto Tracing Ridge Profiles: Wind Turbine Design

This work discovers continuous near-optimal trade-offs between airfoil lift and drag forces by Pareto tracing along a manifold of discrete shapes to augment large scale wind turbine blade inverse problems. Pareto traces constitute curves through parameter space achieving optimal, or near-optimal, trade-offs in bi-criteria optimization. Tracing requires integrating a dynamical system governed by first and second order derivatives of criteria; becoming unstable (or non-existent) if functions do not change significantly (or at all) over parameter combinations in the Cartesian product. Exploring this impasse, we introduce a class of ridge approximations restricting integration over fewer coordinates of reduced dimension subspaces where criteria change the most, on average.

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MS209

Alleviating the Cost of Bayesian Calibration with Embedded Model Error Using Gaussian Process Surrogates and Multilevel Mcmc

Atomistic simulations are commonly used in a variety of energy-related applications. To maintain computational tractability, these simulations often rely on interatomic potentials to rapidly compute potential energies across large collections of atoms. Frequently used potentials – such as those derived through the embedded atom method (EAM) are constructed based on simple "physically-inspired' functional forms and contain unknown parameters that must be fitted to reference data. Prior works have shown Bayesian calibration to be effective for fitting interatomic potential models and quantifying uncertainties in their predictions. Many of these strategies, however, utilize output-additive forms of model error, which can be problematic in the context of predicting new quantities of interest. In the present work, we explore Bayesian calibration with embedded forms of model error in which statistical error terms are embedded directly within the potential model. To alleviate the computational burden levied by this approach, we propose a framework involving surrogate models of multiple fidelities. We leverage sparse Gaussian process techniques to construct a hierarchy of increasingly accurate but more expensive surrogate models. This hierarchy can then be exploited by multilevel Markov chain Monte Carlo methods to efficiently sample from the posterior distribution. We illustrate this approach by calibrating an EAM potential for a family of gold-copper alloys.

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MS209

Adjoint Monte Carlo Sensitivities for Nuclear Fusion Using Reversible Random Number Generators

Tokamak nuclear fusion reactors have the potential to be a clean, reliable source of energy for the future. The design of such a reactor, requires multiple physical phenomena to be taken into account, necessitating expensive computational simulations as part of a PDE-constrained optimization problem. We focus on the simulation of neutral particles in the so-called scrap-off-layer at the edge of the reactor. The kinetic equations modeling these particles are typically simulated using particle-based Monte Carlo methods, which introduce noise to the simulation outputs and, consequently, the objective function being minimized. In this setting, computing the gradient of the objective function to its design parameters requires care to ensure convergence. The discrete-adjoint method computes the gradient through a simulation that retraces the original particle trajectories backwards in time. However, for complex simulations, storing these trajectories requires a large amount of memory. In this work, we tackle this memory issue, by recomputing the reversed trajectories from scratch. To this end, we use a reversible random number generator, i.e., one that can step both forwards and backwards through the random sequence at identical cost. We demonstrate that this approach significantly reduces the memory required in a straightforward implementation of such simulations. We do so on both mathematical toy-problems as well as a simplified reactor edge simulation.

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MS209

Equipping Neural Network Closure Models with Uncertainty for Propagation through High-Fidelity

Simulations

Coarse-grained or filtered models typically rely on closure models to account for unresolved scales. For instance, large eddy simulation for modeling turbulent fluid flows explicitly resolves the largest scales, but requires modeling closure terms to account for the sub-filter scales. With the vast amount of data available from high-fidelity simulations, there are unique opportunities to leverage data-driven modeling techniques to formulate expressive and flexible closure models. Despite their flexibility, data-driven models struggle in domain shift settings, i.e. when deployed in configurations not captured in the training dataset. In particular, the efficacy of neural network surrogates is difficult to assess a priori due to the deterministic, point-estimate nature of predictions. In high-consequence applications, such models require reliable uncertainty estimates in the data-informed and out-of-distribution regimes. To quantify uncertainties in both regimes, we employ Bayesian neural networks which are able to capture both epistemic and aleatoric uncertainties. We will discuss challenges associated with the training and evaluation of these networks. Furthermore, we will discuss uncertainty embedding strategies to enable efficient sampling and propagation of uncertainty through high-fidelity simulations.

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MS210

Bayesian Design of Measurements for Magnetorelaxometry Imaging

The aim of magnetorelaxometry imaging is to determine the distribution of magnetic nanoparticles inside a subject by measuring the relaxation of the superposition magnetic field generated by the nanoparticles after they have first been aligned using an external activation magnetic field that has subsequently been switched off. This work applies techniques of Bayesian optimal experimental design to selecting the positions for the activation coil to increase the value of data and enable more accurate reconstructions. Both Gaussian and total variation prior models are considered for the distribution of the nanoparticles. The former allows simultaneous offline computation of optimized designs for multiple consecutive activations, while the latter introduces adaptability to the algorithm by using previously measured data in choosing the position of the next activation. The total variation prior has a desirable edge-enhancing characteristic, but with the downside that the computationally attractive Gaussian form of the posterior density is lost. To overcome this challenge, the lagged diffusivity iteration is used to provide an approximate Gaussian posterior model and allow the use of the standard Bayesian A- and D-optimality criteria for the total variation prior as well. Two-dimensional numerical experiments are performed on a few sample targets in a simplified setting.

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MS210

Accelerating MCMC for UQ in Imaging Science by Relaxed Proximal-point Langevin Sampling

In this work, we present a highly efficient gradient-based Markov chain Monte Carlo methodology to perform Bayesian computation in in imaging inverse problems with an underlying convex geometry. The proposed strategy takes the form of a stochastic relaxed proximal-point iteration. For models that are smooth or regularised by Moreau-Yosida smoothing, the algorithm is equivalent to an implicit midpoint discretisation of an overdamped Langevin diffusion targeting the posterior distribution of interest. This discretisation is asymptotically unbiased for Gaussian targets and shown to converge in an accelerated manner for any target that is k-strongly log-concave (i.e., requiring in the order of square root k iterations to converge, similarly to accelerated optimisation schemes), comparing favourably to [M. Pereyra, L. Vargas Mieles, K.C. Zygalakis, SIAM J. Imaging Sciences, 13,2 (2020), pp. 905-935] which is only provably accelerated for Gaussian targets and has bias. For targets that are k-strongly log-concave, the provided non-asymptotic convergence analysis also identifies the optimal time step which maximizes the convergence speed. The proposed methodology is demonstrated through a range of experiments related to image deconvolution with Gaussian and Poisson noise, with assumption-driven and data-driven convex priors. The corresponding pre-print is available at ¡a href=https://arxiv.org/abs/2308.09460¿https://arxiv.org/abs/2308.09

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MS210

Variable Step Size SDE for Weak Approximation of Langevin Dynamic

The work focuses on weak approximation of stochastic differential equations and develops a method of computing solutions of Langevin dynamics using variable stepsize. The method assumes a knowledge of the problem allowing to establish a good monitor function which locates points of rapid change in solutions of stochastic differential equations. Using time-transformation we show that it is possible to integrate a rescaled system using fixed-stepsize numerical discretization effectively placing more timesteps where needed.

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MS210

Optimal Approximation Error Approach in Bayesian Inverse Problems

In this presentation, we explore how to mitigate errors when reducing computational cost in high-dimensional Bayesian inverse problems by introducing surrogate forward models. We focus on the Approximation Error Model, which adjusts the likelihood distribution to compensate for the approximation error. The key challenge is selecting the appropriate noise covariance in the Approximation Error Model, which we address by minimizing the distance between the true and approximate posterior distributions averaged over the evidence distribution.

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MS211

Finding a Reduced Data Set for Clinical Time Series Summarization

With bedside monitors continuously displaying and/or recording waveforms to inform patient treatment, the rapid, real-time interpretation of every collected data point in the hospital setting is not a realistic expectation of clinicians. In effort to help distill the large amounts of data—particularly electrocardiogram data—produced over time, this work explores the application of deep learning techniques for noise detection and subset selection techniques for subsequent beat morphology summarization. The evaluated noise detection methods are largely centered around variational autoencoders, and subset selection in the class identification context is evaluated for methods such as leverage scores, the discrete empirical interpolation method (DEIM) (more commonly used in the model reduction context), and variants thereof. Applying these methods to real electrocardiogram data, this multi-faceted approach offers a framework for waveform summarization to help streamline information for clinical decision support.

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MS211

Inference of Ecological Interactions in Stochastic Population Dynamics Models

Ecological interactions between individuals play an important role in the evolutionary dynamics of the whole population. In this talk, I will discuss methods to infer interaction mechanisms underlying time-series data from a sequence of three population systems that increase in scale: (1) homogenous populations, (2) two-phenotype heterogenous populations, (3) networks of many-phenotype heterogeneous populations. The discussion on each of these population scales draws from my work on three separate projects, each of which highlights the role of demographic stochasticity in parameter identifiability and estimation. In the first project on homogenous populations joint with Peter Thomas (Case Western Reserve University) and Jacob Scott (Cleveland Clinic), we infer whether competitive interactions happen through the birth process, the death process, or a combination of the two. The second project on two-phenotype heterogenous populations is an extension of the first project and joint with Heyrim Cho (UC Riverside) and Erin Beckman (Utah State University). We infer birth vs. death regulation of three types of interactions: competitive, cooperative, and antagonistic. The last project was developed at the 2023 AMS MRC workshop led by Heather Zinn Brooks (Harvey Mudd College) and Phil Chodrow (Middleburry College). Together with Heather and Phil, we (Tom Gebhart, Linh Huynh, Vicki Modisette, Will Thompson, Moyi Tian) have inferred interaction kernels in stochastic agent-based systems.

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MS211

Modeling and Tracking Random Motion in Micrometer-Scale Living Systems

We study stochastic motion of objects in micrometer-scale living systems: tracer particles in living cells, pathogens in mucus, and single cells foraging for food. We use stochastic models and state space models to track objects through

time and infer properties of objects and their surroundings. For example, we can calculate the distribution of first passage times for a pathogen to cross a mucus barrier, or we can spatially resolve the fluid properties of the cytoplasm in a living cell. Recently developed computational tools, particularly in the area of Markov Chain Monte Carlo, are creating new opportunities to improve multiple object tracking. The primary remaining challenge, called the data association problem, involves mapping measurement data (e.g., positions of objects in a video) to objects through time. I will discuss new developments in the field and ongoing efforts in my lab to implement them. I will motivate these techniques with specific examples that include tracking salmonella in GI mucus, genetically expressed proteins in the cell cytoplasm, active transport of nuclei in multinucleate fungal cells, and raphid diatoms in seawater surface interfaces.

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MS211

Data Driven Modeling of Biological Systems Using DNN

We present a data driven method for modeling of unknown dynamical systems in mathematical biology. The method is designed to discover the flow map operator behind the data and utilize deep neural network (DNN) as the main numerical technique for the discovery. Once an accurate DNN model for the flow map is constructed, it serves as a predictive model for the unknown system and enables us to conduct long-term system prediction and analysis. The method is highly versatile and can be applied to non-autonomous systems, systems with missing variables and/or hidden parameters.

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MS212

Sequential Design for Hierarchical Models

When we have models that need Exascale computation (10^{18} flops) we cannot do uncertainty quantification solely on the Exascale machine as the runs will be too expensive. One solution to this problem is to in a hierarchy of different levels of complexity ranging from the very basic to the Exascale. To make use of runs over all levels, and crucially improve predictions at the topmost level, we use multi-level Gaussian process emulators (GPs). The accuracy of the GP greatly depends on the design of the training points. Not only the design at each level but across the hierarchy as well. We present a multi-level adaptive sampling algorithm to sequentially increase the set of design points to optimally improve the fit of the GP. The normalised expected leave-one-out cross-validation error is calculated at all unobserved locations, and a new design point is chosen using expected improvement combined with a repulsion function. This criterion is calculated for each model level weighted by an associated cost for running the code at that level. Hence, at each iteration, our algorithm optimises for both the new point location and the level at which the model is run at. The algorithm is extended to batch selection as well as single point selection, where batches can be designed for single levels or optimally across all levels.

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MS212

UQ for High-dimensional Uncertain Parameter Spaces: the Case of Classical Molecular Dynamics

Uncertainty quantification (UQ) is essential for computational science and engineering applications from which actionable outcomes are anticipated. Many real world applications involved large numbers of parameters and are out of scope for standard UQ approaches which suffer from the curse of dimensionality. New developments based on active subspaces that invoke machine learning, kernel methods and Gaussian processes now allow allow us to implement scalable solutions that can assess the uncertainties arising from the sensitivity of the input parameters is ranked. In this paper, we report a study of classical molecular dynamics with a particular focus on uncertainties in the high-dimensional force-field parameters, which affect key quantities of interest, including advanced materials properties and binding free energy predictions in drug discovery. Our analyses reveal that the prediction uncertainty is dominated by a small number of the hundreds of interaction potential parameters within the force fields employed. This ranking is of immediate scientific interest since it reveals those interactions which control the prediction uncertainty, thereby facilitating systematic improvements to be made in the optimisation of molecular dynamics forcefields.

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MS212

Scalable Uncertainty Quantification with the SEAVEA toolkit

Computer-based simulations have become a critical component of many fields of scientific research and well beyond. The availability of supercomputers permits studies on topics of major societal importance, including climate change, medicine, and energy production, conducted at ever-increasing scales and scope. As such it is important to equip the output data with meaningful bounds on errors which come from rigorous uncertainty quantification (UQ), which invariably requires running model ensembles on supercomputers. Within the context of the Software Environ-

ment for Actionable VVUQ-evaluated Exascale Applications (SEAVEA) toolkit we will highlight several UQ methods for scalable UQ, both from a methodological and high-performance computing point of view. The focus of this talk will be on real-world models with high-dimensional parameter spaces, and how one can use SEAVEA toolkit components to quantify their uncertainty.

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MS212

A New Bayesian Method for Building Gaussian Process Emulators from Hierarchies of Models

Decision making often uses complex computer codes run at the exa-scale (10e18 flops). Such computer codes or models are often run in a hierarchy of different levels of fidelity ranging from the basic to the very sophisticated. The top levels in this hierarchy are expensive to run, limiting the number of possible runs. To make use of runs over all levels, and crucially improve emulation at the top level, we use multi-level Gaussian process emulators (GPs). We will present a new method of building GP emulators from hierarchies of models. In order to share information across the different levels, $l = 1, , L$, we define the form of the prior of the $l + 1^{\text{th}}$ level to be the posterior of the l^{th} level, hence building a Bayesian hierarchical structure for the top Lth level. This enables us to not only learn about the GP hyperparameters as we move up the multi-level hierarchy, but also allows us to limit the total number of parameters in the full model, whilst maintaining accuracy. As well as providing details of the methodology, we will also present several examples. This includes comparisons to well-known alternatives, and a demonstration of how our method is effective with very few (only 1 or 2) runs of the expensive top levels of the model. Lastly, we discuss whether the predicted variance of a multi-level GP should increase as we include more data on the top levels.

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MS213

Projected Ensemble Data Assimilation

Ensemble data assimilation is unable to reduce the error estimate for high-dimensional systems when used with small ensemble size. A typical remedy is dimesion reduction by localization. Though localization reduces the error substantially for both linear and nonlinear data-assimilation methods, the former ones considerably outperform the latter ones in a quasi-linear regime. We propose a further dimension reduction based on projection and show substantial error decrease of a nonlinear data-assimilation method in a challenging data-assimilation numerical setup with small ensemble size and ample observations.

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MS213

Observer-Based Data Assimilation for Barotropic Euler Equations

We consider a state estimation problem for a system described by nonlinear hyperbolic conservation laws, more precisely, by the one-dimensional barotropic Euler equations as a model for gas transport through gas pipes. For this system, we construct an observer system of Luenberger type that is based on distributed measurements of one state variable. Writing the system in a Hamiltonian formulation allows us to use an extension of the relative energy method in order to show that the state of the observer system converges for long times exponentially fast towards the original system state. Using energy-conserving coupling conditions at the pipe junctions the results can be extended to star-shaped networks.

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MS213

Observability and Filtering

In applying any practical data assimilation algorithm, an often implicit assumption is the observability (or detectability) of the hidden process. In this talk, I will provide a brief historical review of observability noting the important contributions over the years (1960-present). Next, I will describe some recent definitions of observability based on the duality between filtering and optimal control. I will relate these definitions to the question of filter stability and discuss some open problems related to the stability of various types of particle approximations of the filter.

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MS213

Stepwise Data Absorption Combining Complementary Filtering Techniques

Data Assimilation serves multiple purposes, including estimating the model state and the initial state of a system for predicting its future state. It combines prior information from numerical model simulations with observed data to produce the most accurate description of a dynamical system and its uncertainty. Here we introduce additional importance sampling steps by splitting the likelihood in order to improve the robustness and accuracy of the estimations. This approach allows us to combine Gaussian approximative filters such as the Ensemble Square Root Filter (ESRF) and consistent filters such as the Ensemble Transform Particle Filter (ETPF). The benefit is that one can exploit the stabilizing properties of ESRF type filters while mimicking the accuracy level of a consistent filter.

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MS214

Gaussian Process Regression in Inverse Problems and Markov Chain Monte Carlo

We are interested in the inverse problem of estimating unknown parameters in a partial differential equation from observed data. Solving inverse problems by the Bayesian approach gives a distribution of the unknown parameters conditioned on the observed data, which is often in high dimensions and difficult to extract information from. Sampling methods such as Markov chain Monte Carlo are popular choices, but the major challenge in their applications is then the huge computational cost associated with repeatedly solving the PDE with different parameter values. To overcome this issue, we consider using Gaussian process regression (GPR) to approximate the likelihood of the data. This results in an approximate posterior distribution, to which sampling methods can be applied with feasible computational cost. In this talk, we will show how the uncertainty estimate provided by GPR can be incorporated into the approximate Bayesian posterior distribution to avoid overconfident predictions, how the PDE constraints can be incorporated into the prior of GPR to obtain a physics-informed model, and present efficient Markov chain Monte Carlo methods in this context.

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MS214

Gaussian Processes-Based Estimation of Derivatives

In this presentation, we introduce a novel method for estimating derivatives of multivariate 1D functions that are only accessible through noisy observations. We begin by fitting a Gaussian process (GP) model to the observations augmented with stencil points centered around them. The derivatives are then estimated by predicting function values at stencil points and by computing finite difference approximations given these values. Because our method is GP-based, it inherently provides uncertainty quantification on the derivatives approximations. We validate our approach on simulated data and highlight how it can be leveraged to accelerate Bayesian optimization-type algorithms.

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MS214

Linear Methods for Non-Linear Inverse Problems

We consider recovering an unknown function f from a noisy observation of the solution u_f to a partial differential equation of the type $\mathcal{L}u_f = c(f, u_f)$ for a differential operator $\mathcal{L}$, and invertible function c, i.e. $f = e(\mathcal{L}u_f)$. Examples include amongst others the time-independent Schrödinger equation $\frac{1}{2}\Delta u_f = u_f f$ and the heat equation with absorption term $\frac{du_f}{dt} - \frac{1}{2}\Delta u_f = f$. We transform this problem into the linear inverse problem of recovering $\mathcal{L}u_f$ under Dirichlet boundary condition, and show that Bayesian methods (with priors placed either on u_f or $\mathcal{L}u_f$) for this problem may yield optimal recovery rates not only for u_f, but also for f. We also derive frequentist coverage guarantees for the corresponding Bayesian credible sets. Adaptive priors are shown to yield adaptive contraction rates for f, thus eliminating the need to know the smoothness of this function. The results are illustrated by several numerical analysis on synthetic data sets.

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MS215

Sensitivity Analysis of Set-Valued Models. Application to Sensitivity Analysis of Pollutant Concentration Maps

In the context of air quality control, we are interested in measuring the influence of uncertain inputs on pollutant dispersion maps. Using sensitivity analysis methods, we aim to quantify the influence of five inputs to a meta-model of pollutant concentration maps in the urban area of Issy-Les-Moulineaux. However, most sensitivity analysis methods deal with scalar or vectorial outputs. A map-valued output space makes the adaptation of classical sensitivity analysis methods non-trivial. We propose to consider the maps as sets and to perform sensitivity analysis on a set-valued model. In a general framework of set-valued models, we propose to use kernel-based sensitivity analysis and, in particular, HSIC-based indices. We use a kernel between

sets, and we show that it is *characteristic* (i.e. injectivity of the embedding in the associated Reproducing Kernel Hilbert Space), a necessary property to use the HSIC in a sensitivity analysis context. We then propose to compute HSIC-ANOVA indices that allow a decomposition of the input contributions. Using these indices, we can identify which inputs should be neglected (*screening*) and we can rank the others according to their influence (*ranking*). The estimation of these indices is also adapted to the set-valued outputs. Finally, we test the proposed method on the model of pollutant concentration maps.

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MS215

Global Reliability Sensitivity Analysis of Systems with Multiple Failure Modes

Global variance-based reliability sensitivity measures arise from a variance decomposition of the indicator function describing the failure event. The first-order indices reflect the main effect of each variable on the variance of the failure event and can be used for variable prioritization; the total-effect indices represent the total effect of each variable, including its interaction with other variables, and can be used for variable fixing. This contribution derives expressions for the variance-based reliability indices of systems with multiple failure modes that are based on the first-order reliability method (FORM). The derived expressions are a function of the FORM results and, hence, do not require additional expensive model evaluations. They do involve the evaluation of multinormal integrals, for which effective solutions are available. We demonstrate that the derived expressions enable an accurate estimation of variance-based reliability sensitivities for general system problems.

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MS215

Elastic Sensitivity: Higher Order Effects Via Search Curves - A Comparison

Numerical models for assessing the safety of repositories for radioactive waste can be highly nonlinear with respect to their input parameters, showing phenomena like non-monotonicity, discontinuity, and multimodality. The output distributions can span several orders of magnitude and exhibit high skewness. Parameter interactions often play an important role for the model behavior. Higher-order sensitivity analysis quantifies such interactions and can provide valuable information about the system under investigation. This, however, is a challenging task. Metamodeling approaches like Random-Sampling High Dimensional Model Representation (RS-HDMR) or polynomial chaos expansion (PCE) are a well-approved means but may require many model runs and may be susceptible to overfitting artifacts. The FAST sensitivity method traverses the input space along a curve with a specified frequency behavior. We mimic this approach in a given data context by introducing suitable search curves to transfer lower dimensional projection of the input space into a one-dimensional setting, allowing for the use of spectral-type sensitivity indicators or of mean square successive differences (Chatterjee-type) estimators on the reordered outputs. We demonstrate the approach in comparison with RS-HDMR and PCE by application to a realistic repository model with various nonlinear properties.

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MS215

Quantile Oriented Sensitivity Analysis Index Estimation Based on Random Forests

In this work, we are interested in quantile oriented sensitivity analysis (QOSA). The aim of QOSA is to quantify feature importance at different quantile level of a scalar response variable. We propose here to estimate QOSA indices [Fort et al., 2016] (see also [Maume-Deschamps and Niang, 2018]) using random forests. Following [Elie-Dit-Cosaque and Maume-Deschamps, 2021], we propose an estimation procedure based on random forests. We first build a quantile oriented random forest by splitting criterion in [Bhat et al., 2015], as an alternative to generalized random forests introduced in [Athey et al., 2019]. Then, following [Bnard et al., 2022], we estimate QOSA indices based on projected random forests. The performances of our esti-

mation procedure are tested on simulated data.

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MS216

Rethinking Bayesian Active Learning

Bayesian active learning involves seeking the most informative labels for training a predictive model. We argue that two aspects of its predominant implementation need rethinking. First, whereas the literature has historically focused on maximally reducing parameter uncertainty, we advocate targeting predictive uncertainty on an input distribution of interest. Second, we recommend a shift towards semi-supervised models in order to capitalise on the abundant information often present in unlabelled data. We demonstrate that these two changes are crucial in making Bayesian active learning more useful in modern machine learning, where we often work with high-dimensional inputs, uncurated pools of unlabelled data and flexible predictive models.

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MS216

Multifidelity Bayesian Optimal Experimental Design

Mathematical models of engineering phenomena are vital for prediction, design, and control. In many cases, these models have uncertain parameters that must be inferred from experimental data. However, experiments may be costly, time-demanding, or even dangerous. As such, it is often important to identify conditions that maximize the value of experiments. Model-based optimal experimental design (OED) provides a rigorous framework for identifying the ideal experimental design by leveraging a mathematical model that simulates the experimental outcomes. In this work, the value of an experiment is quantified via the expected information gain (EIG), which is typically estimated numerically using double-nested Monte Carlo (DNMC). The nested loops in DNMC can be prohibitively expensive for compute-intensive models. We propose a multi-fidelity acceleration, in which an ensemble of EIG estimators of varying accuracy and cost (e.g. from lower-fidelity models that use simplified physics, coarsened meshes, or partial convergence) are combined via the approximate control variate method. By leveraging many evaluations of the low-fidelity model(s) and few of the highest-fidelity model, the multi-fidelity estimator achieves lower variance while remaining unbiased. This approach is demonstrated on a nonlinear benchmark and in designing flow experiments for inferring the Reynolds-averaged NavierStokes (RANS) turbulence closure model parameters.

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MS216

Uncertainty Quantification in Neural Networks is a Bottleneck for Inverse Molecular dDesign

Chemical space - the total number of molecules that could be made - is astronomically large and finding optimal chemicals for a desired application in therapeutics, sustainability or other applications requires extensive iterations. Generative models in molecular applications can power molecular design by automatically suggesting highly promising candidates. In the last decade, an increasing number of powerful algorithms have been proposed to sample molecules that satisfy some desired properties, from reinforcement learning to generative adversarial networks and variational auto encoders to diffusion-based models. However, most models struggle to discover new molecules that are useful because of the poor generalizability of the scoring functions that predict molecular properties and thus guide the design. Active learning is typically the proposed path to building robust, generalizable property prediction functions that can power the design of novel, highly promising chemicals. Here, we will describe our current work in uncertainty quantification of machine learning property prediction models through single-model (mean-variance estimation, latent-space distance, deep evidential regression) and ensemble techniques. We will evaluate their ability to quantify epistemic and aleatoric uncertainty and enable active learning in the training of machine learning interatomic potentials.

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MS216

Distributionally Robust Nearest-Neighbor Selection to Inform Action Recommendations

I will start by presenting a distributionally robust optimization approach to learning predictive models, using general loss functions that can be used either in the context of classification or regression. Motivated by applications in health care, we consider a setting where training data may be contaminated with (unknown) outliers. The robust learning problem is formulated as the problem of minimizing the worst case expected loss over a family of distributions that are close to the empirical distribution obtained from the training data. We will explore the generality of this approach, its robustness properties, its ability to explain a

host of "ad-hoc" regularized learning methods, and we will establish rigorous out-of-sample performance guarantees. I will then discuss how this framework can be used to to make decisions and offer specific personalized prescriptions and recommendations to improve future outcomes. I will discuss a particular application in making treatment recommendations for hypertension.

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MS217

Some Theoretical Aspects of Particle Filters and Ensemble Kalman Filters

In the last three decades, Particle Filters (PF) and Ensemble Kalman Filters (EnKF) have become one of the main numerical techniques in data assimilation, Bayesian statistical inference and nonlinear filtering. Both particle algorithms can be viewed as mean field type particle interpretation of the filtering equation and the Kalman recursion. In contrast with conventional particle filters, the EnKF is defined by a system of particles evolving as the signal in some state space with an interaction function that depends on the sample covariance matrices of the system. Despite widespread usage, little is known about the mathematical foundations of EnKF. Most of the literature on EnKF amounts to design different classes of useable observer-type particle methods. To design any type of consistent and meaningful filter, it is crucial to understand their mathematical foundations and their learning/tracking capabilities. This talk discusses some theoretical aspects of these numerical techniques. We present some recent advances on the stability properties of these filters. We also initiate a comparison between these particle samplers and discuss some open research questions

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MS217

High Dimensional Ensemble Kalman Inversion with Dropout

Ensemble Kalman inversion (EKI) is an ensemble-based method to solve inverse problems. Its gradient-free formulation makes it an attractive tool for problems with involved for- mulation. However, EKI suffers from the subspace property, i.e., the EKI solutions are confined in the subspace spanned by the initial ensemble. It implies that the ensemble size should be larger than the problem dimension to ensure EKIs convergence to the correct solution. Such scaling of ensemble size is impractical and prevents the use of EKI in high dimensional problems. To address this issue, we propose a novel approach using dropout regularization to mitigate the subspace problem. We prove that dropout-EKI converges in the small ensemble settings, and the computational cost of the algorithm scales linearly with dimension. We also show that dropout-EKI reaches the optimal query complexity, up to a constant factor. Numerical examples demonstrate the effectiveness of our approach.

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MS217

Operator Learning for Stochastic Closures of Complex Dynamical Systems

Closure models are widely used in simulating complex multiscale dynamical systems such as turbulence and Earths climate, for which direct numerical simulation that resolves all scales is often too expensive. For those systems without a clear scale separation, deterministic and local closure models often lack enough generalization capability, which limits their performance in many real-world applications. In this talk, we present a data-driven modeling framework for constructing stochastic and nonlocal closure models from (i) abundant data, and (ii) a limited amount of data. Specifically, operator learning with indirect data will be demonstrated in the context of stochastic differential equations. We also show how different types of regularization can be imposed to improve the performance of the learned closure models. The results show that the proposed methodology provides a systematic approach to constructing generalizable data-driven closure models for multiscale dynamical systems even if there is no clear scale separation between resolved and unresolved scales.

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MS217

Bayesian Inference Using Self-Reinforced Sum-of-Squares

Our work addresses the challenging task of approximating and sampling from a highly concentrated posterior density known up to a normalizing constant. We present a novel variational density approximation technique employing Sum-of-Squares (SoS) functions as the approximation tool. Notably, SoS preserve the convexity properties of the statistical divergence employed in the inference process. Furthermore, this approximation tool allows for the construction of triangular transports through the Knothe-Rosenblatt rearrangement. To approximate such complex densities efficiently, we employ a recently proposed greedy approach known as "self-reinforcement". This method dissects the highly concentrated density into a sequence of intermediary densities, reducing the complexity of the estimation task. We establish an error bound for our method by leveraging α-divergences, a class of divergences encompassing the KL-divergence, Hellinger distance, and χ^2-divergence, within the variational framework. To demonstrate the practical effectiveness of our approach, we provide numerical examples showcasing its performance and robustness in Bayesian inference tasks.

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MS218

Reduced Order Models for the Finite Element Approximation of Eigenvalue Problems

Following [1], we consider a reduced order method for the approximation of the eigensolutions of the Laplace problem. Using a time continuation technique that consists in the introduction of a fictitious time parameter, a POD approach is developed. Particular importance is given to the choice of the dimension of the POD basis, leading to optimal behavior of the approximate solution. This approach lead to a data-driven reduced basis method for the approximation of parametric eigenvalue problems, based on the offline and online paradigms, see [2]. In the offline stage, snapshots are generated and construct the basis of the reduced space. Gaussian process regressions can be used for approximating the eigenvalues and projection coefficients of the eigenvectors in the reduced space. All the GPR corresponding to the eigenvalues and projection coefficients are trained in the offline stage, using the data generated in the offline stage while the output corresponding to new parameters is obtained in the online stage. Numerical results for the solution of affine and non-affine parameter-dependent eigenvalue problems demonstrate the robustness of the non-intrusive method. [1] FB, D. Boffi, A. Halim, A reduced order model for the finite element approximation of eigenvalue problems, Computer Methods in Applied Mechanics and Engineering, 404 (2023) [2] – Data-driven reduced order modeling for parametric PDE eigenvalue problems using Gaussian process regression, to appear in JCP

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MS218

Nonlinear Reduced Basis Using Mixture Wasserstein Barycenters: Application to an Eigenvalue Problem Inspired from Quantum Chemistry

We are interested in the computation of the ground state of a molecular system with nuclei characterized by their positions in space and their electric charges. The ground state is the solution to a (possibly nonlinear) eigenvalue problem, called Shrdinger equation. Solutions are mostly computed as a linear combination on a well-chosen basis, but solving this problem for many different geometries can be costly, as in molecular dynamics and geometry optimization. In this talk, I will focus on a 1D Schrdinger equation, for which analytic solutions are fully characterized [Pham, Galerkin method using wavelet-Gaussian bases...]. In the following, we propose a new approach based on an interpolation method, called mixture Wasserstein barycenters. It relies heavily on the shape of the solutions (called mixtures) and on the Wasserstein metric, but contrary to Wasserstein barycenters, can be computed efficiently and is expected to scale to higher dimensions [Delon and Desolneux, A wasserstein-type distance in the space of gaussian mixture models] [Dusson, Ehrlacher, and Nouaime, A wasserstein-type metric for generic mixture models...]. First, we make use of a greedy algorithm to choose the few representative solutions we want to interpolate with. Then, we will see how to compute optimal parameters representing the current solution as an interpolation of selected solutions. We will also present some numerical results, and some hints on how to scale to higher dimensions.

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MS218

On Uncertainty Quantification of Eigenpairs with Higher Multiplicity

We consider generalized operator eigenvalue problems in variational form with random perturbations in the bilinear forms. This setting is motivated by variational forms of partial differential equations with random input data. The considered eigenpairs can be of higher but finite multiplicity. We investigate stochastic quantities of interest of the eigenpairs and discuss why, for eigevalues of multiplicity greater than 1 in some parts of the parameter space, only the stochastic properties of the eigenspaces are meaningful, but not the ones of individual eigenpairs. To that end, we characterize the Frchet derivatives of the eigenpairs with respect to the perturbation and provide a new linear characterization for eigenpairs of higher multiplicity. For the uncertainty quantification of eigenspaces we consider meaningful sampling strategies as well as perturbation approaches. Numerical examples are presented to illustrate the theoretical results.

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MS218

Stochastic Collocation Method for Computing

Eigenspaces of Parameter-Dependent Operators

We consider computing eigenspaces of an elliptic self-adjoint operator depending on a countable number of parameters. We restrict our study to the problems where this dependence on parameters has an affine structure and assume that the cluster (collection) of eigenvalues which we track satisfies the spectral gap condition. Precisely, this means that we assume that the collection of eigenvalues is separated from the rest of the spectrum for all values of parameters. We show that the associated parameter dependent family of eigenprojections can be extended to complex-analytic functions of the parameters. Based on this result we provide error estimates and show that this leads to convergence of sparse polynomial approximations. Starting with this analytic family of projections we construct a stochastic collocation method for computing a parameter dependent basis for the eigenspace of interest. We evaluate and verify the methods in a series of numerical experiments for a stochastic diffusion operator.

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MS219

Calibrating and Optimizing Operator Term via a Neural Galerkin Projection on the Shallow Water Equations

Successful reduced order models (ROMs) can enable a computationally inexpensive framework for quickly modeling partial differential equations (PDEs). With Galerkin Projection ROMs (GPROMs), a system of PDEs are turned into a system of ordinary differential equations (ODEs) by representation of the state as an expansion into a reduced-dimension, orthogonal basis, which is then projected back onto the PDEs. However, GP-ROMs have particular difficulty predicting long-time dynamics, typically as selection of a reduced-order basis removes important interaction of higher modes. The GP-ROMs can be calibrated, for example, by basis-weighting methods or by introducing scaling terms in the ODEs, but this can often be difficult and is highly problem specific. Alternatively, neural networks can learn calibration terms directly from the data and optimize them, as in the recent work solving compressible Navier-Stokes GP-ROMs with differentiable programming [1]. In this work, we extend these methods to the shallow water equations (SWE). We show by training and parameterization on SWE simulations, its long-time stability and accuracy dynamics are significantly improved at a low computation cost, thereby empowering rapidly deployable solutions for urgent forecasting problems.

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MS219

Budget-Limited Calibration of Computationally Expensive Physical Models

While parameter estimation methods for complex physical models are well-established, these tools often remain far out of the reach for many engineering problems due to the computationally expensive nature of the underlying models. The situation is typically far worse in settings where we also wish to estimate associated posterior distribution via Markov Chain Monte Carlo. In this work we present an approach which seeks to overcome this challenge by making judicious use of surrogate modelling and Bayesian experimental design. More specifically, we investigate Bayesian posterior inference in budget-limited settings where the likelihood can only be computed a fixed number of times. We reformulate posterior inference as a sequential Bayesian experimental design problem. The unknown forward problem is characterised by a surrogate model, which is sequentially updated, along with with an ensemble of particles whose distribution will converge to the associated posterior distribution / MAP estimator. We show that this approach provides an effective approach to approximate posterior inference for computationally challenging Bayesian inverse problems arising in physics and engineering.

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MS219

Physics-Driven Deep Latent Variable Models : Solving Forward and Inverse Problems in Parametric PDEs

We introduce a physics-driven deep latent variable model (PDDLVM) to simultaneously learn parameter-to-solution (forward) and solution-to-parameter (inverse) maps of parametric partial differential equations (PDEs). Our formulation leverages conventional PDE discretization techniques, deep neural networks, probabilistic modelling, and variational inference to assemble a fully probabilistic coherent framework. The model is trained by maximizing the evidence lower bound (ELBO) of a zero-valued residual. Consequently, the proposed methodology does not require any independent PDE solves and is physics-informed at training time, allowing the real-time solution of PDE forward and inverse problems after training. We demonstrate the efficiency and robustness of our method on finite element discretized parametric PDE problems such as linear and nonlinear Poisson problems, elastic shells with complex 3D geometries, and time-dependent nonlinear and inhomogeneous PDEs.

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MS221

SA UQ in Hemodynamics Modeling for Liver

Surgery

Major liver resection is a surgical procedure consisting of the removal of a significant portion of liver tissue, and is considered the only curative treatment of primary or secondary liver tumors. Removal of liver tissue significantly alters hepatic hemodynamics (i.e., pressure and flows in liver circulation) and may lead to post-operative portal vein hypertension (PHT) and ultimately, death. Recently, our group has shown the feasibility of using lumped parameter models to integrate clinical measurements and predict post-operative portal vein pressure on a patient basis. However, clinical data is sparse and noisy, which should be reflected in model-based predictions. Furthermore, we rely on invasive data obtained during surgery, which is contradictory to the concept of pre-operative prediction. We first performed a sensitivity analysis using sparse polynomial chaos expansion to prioritize the set of model input parameters required for personalization of the hemodynamics model. Optimization is performed using a covariance matrix adaptation evolution strategy. To ensure a unique solution to the optimization procedure, a profile likelihood analysis was performed, which lead to the inclusion of a new clinical measurements. Finally, we used PCE to generate the final patient specific UQ. In future work, we aim to further reduce the amount of invasive input data needed and refine the hemodynamics model to improve the models predictive power.

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MS222

Kernel Methods for Rough Partial Differential Equations

Following the promising success of kernel methods in solving non-linear partial differential equations (PDEs), we investigate the application of Gaussian process methods to solve PDEs with rough right-hand side. We introduce an optimal recovery scheme defined by a Reproducing Kernel Hilbert Space (RKHS) of functions of greater regularity than that of the PDEs solution. We present the resulting theoretical framework and its convergence guarantees for the recovery of solutions to the PDE. We illustrate its application to problems arising from stochastic partial differential equations through numerical experiments.

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MS222

Trustworthy and Scalable Data-Driven Closure Models

Computational simulations of dynamical systems often require constitutive or closure models to represent unresolved phenomena, enhance computational efficiency, or correct model form error in the simulation. Data-driven closure models (DDCMs) employ machine learning (ML) to learn the closure term as a function of dynamic system states and have the potential to increase the predictive capability of computational simulations; however, the trustworthiness of the DDCM prediction and scalability of the DDCM implementation are impediments to current adoption. In this work, we propose a methodology that addresses these limitations. Our approach decouples the estimation of the closure term from training the DDCM for increased scalability. The closure term is estimated from experimental data using ensemble Kalman filters (EnKF), or one of its variants, for increased efficiency, and then training the DDCM occurs offline. For trustworthiness, accurate uncertainty quantification (UQ) for DDCM predictions is essential. Uncertainties that arise from sparse or noisy experimental data are mapped to the estimated closure term using the EKF, and then probabilistic ML algorithms propagate uncertainties to the predicted quantity. We demonstrate our methodology on an exemplar from epidemiological disease transmission. *SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.*

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MS223

Gradient-based Dimension Reduction for Solving Bayesian Inverse Problems

Computational Bayesian inference aims to characterize the

posterior probability distributions for parameters in statistical models. The complexity of many inference methods such as MCMC and variational inference, however, typically scale poorly with the growing dimensions of model parameters and data. A recent approach to deal with high or possibly even infinite-dimensional parameters is to exploit low-dimensional structure in the inverse problem and approximately reformulate it in low-to-moderate dimensions. In this presentation, we will introduce an information-theoretic analysis to bound the error from reducing the dimensions of both parameters and data. This bound exploits gradient evaluations of the log-likelihood function to identify relevant low-dimensional subspaces for these variables as well as reveal reduced dimensions that result in minimal error. The benefit of the proposed dimension reduction technique will be demonstrated using several inference algorithms on applications including image processing and data assimilation for aerodynamic flows.

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MS223

Efficient Time-dependent PDE-constrained Optimization Under Uncertainty via Multiple-Input Operator Networks

In this presentation, we address the challenges of applying the DeepONet architecture to PDE-constrained optimization under uncertainty. While DeepONet has been effective in providing fast surrogates in solving time-dependent PDE-constrained optimization (PDECO) problems [Wang, Sifan, et al. 'Fast PDE-Constrained Optimization via Self-Supervised Operator Learning,' arXiv, 25 Oct. 2021], it encounters limitations in cases where the operator depends on multiple inputs. In PDECO under uncertainty, the solution operator maps the product of two Banach spaces the control space and the uncertain parameter space (e.g., heat conduction field for the heat equation, permeability coefficient for Darcy flow diffusion equation, material property in elasticity equation) to the PDE solution Banach space. To address this challenge, we employ the Multiple Input Operator Network (MIONet) [Jin, Pengzhan, et al. 'MIONet: Learning Multiple-Input Operators via Tensor Product,' SIAM Journal on Scientific Computing, vol. 44, no. 6, Dec. 2022]. MIONet provides a versatile framework for learning surrogate models that can handle operators dependent on multiple inputs. We demonstrate how this surrogate model can be effectively used to optimize risk-averse measures and obtain robust controls under uncertainty.

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MS223

Frchet Derivatives of Expected Functionals of Solutions to Stochastic Differential Equations

The estimation of statistics of functionals of a diffusion process is a problem that arises in multiple applications. In rare event sampling, one may seek to estimate the expected value of the first exit time of a diffusion process from a bounded domain, for example. One approach to estimate such statistics involves importance sampling via a change of measure, where the optimal change of measure is unique and yields a zero-variance estimator. Finding the optimal change of measure can be formulated as a stochastic optimal control problem. We describe some stochastic optimal control problems of this type and analyse the convergence behaviour of some natural gradient-based methods for numerically approximating the solutions of these optimal control problems.

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MS223

Scalable Methods for Computing Sharp Extreme Event Probabilities in Infinite-Dimensional Stochastic Systems

We introduce scalable computational techniques for sharp extreme event probability estimates in stochastic differential equations with small additive Gaussian noise. For that purpose, we extend algorithms based on Laplace's method to infinite dimensional path space. The method estimates the limiting exponential scaling of the probability using a single realization of the process, the large deviation minimizer, solution to an optimization problem governed by a differential equation. The probability estimate becomes sharp after including prefactor information, which necessitates computing the determinant of a second derivative operator to evaluate a Gaussian integral around the minimizer. We present an approach in infinite dimensions based on Fredholm determinants, and develop numerical algorithms to compute these determinants efficiently for the high-dimensional discretized systems. We illustrate the method in examples of stochastic (partial) differential equations, including the stochastically forced incompressible three-dimensional Navier–Stokes equations. The presentation is based on [Schorlepp, T., Tong, S., Grafke, T., & Stadler, G. (2023). arXiv:2303.11919]. If time permits, we will show how our results can be used for improved

importance sampling of extreme events as in [Ebener, L., Margazoglou, G., Friedrich, J., Biferale, L., & Grauer, R. (2019). Chaos 29(6)] and [Tong, S., & Stadler, G. (2023). JUQ 11(3)].

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MS224

Managing Power Grid Outages Driven by Climatic Extremes

We explore, numerically and statistically, the relationship between climate extremes and optimal management of powergrids. We demonstrate our statistical approach using the NREL-118 test system which represents three regions in California and consists of 118 buses, 186 transmission lines and 327 generators with 9 different generation technologies. We use Pyomo to calculate optimal generation schedules under specified demand. Data for the NREL-118 is available in the form of hourly demand and generation over a period of 1 year. We construe daily demand as independent samples from a 24-dimensional random variable . For each of these demand samples we evaluate, using Pyomo, with operational constraints, the optimal hourly generation over each of the 327 generators, together with the associated cost. We set a threshold for extreme scenarios based on critical cost. Our task is to characterize the statistics of these extremes and their dependence on geographic and weather conditions. For that we pursue a nonlinear dimension reduction using diffusion on the graph with 365 vertices. We observe a localization onto a vector space spanned by the dominant subspace of the diffusion matrix. We then carry-out statistical sampling on this manifold. We also identify outliers based on their manifold distance to their neighbors.

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MS224

Reduced-Dimensional Neural Network Surrogate Construction for the E3SM Land Model

Prediction uncertainties in the Energy Exascale Earth System (E3SM) land model (ELM) are caused in part by uncertain parameters related fluxes of carbon and energy. Uncertainty quantification and calibration methods hinge on the development of surrogate models that replicate the ELM output behavior with respect to these uncertain input parameters. A major challenge is the high dimensionality of the output spatio-temporal fields. Here we used Karhunen-Love (KL) expansion to reduce a large number of spatio-temporal outputs to a handful of eigenfeatures or latent variables. Neural network (NN) surrogates were then constructed for all latent variables with respect to model input parameters. We employ Residual NNs with layer-parameterized weights that regularize the training and improve performance in approximating the input-output maps. A KLNN surrogate is developed for gross primary productivity (GPP) and employed for global sensitivity analysis. We then perform Markov-chain Monte Carlo based Bayesian calibration using gridded GPP observations and the KLNN surrogate. We construct Bayesian likelihoods via model/data discrepancy in the KL latent space. We investigate the behavior of the calibrated parameters with respect to plant functional types (PFTs). We demonstrate the surrogate construction and calibration for ELM with 275 training simulations at 2x2degree spatial and monthly temporal resolution over a 15-year time period while perturbing 10 model parameters.

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MS224

Working Towards Dark Target Aerosol Product Synergy Among Geo and Leo Sensors An Uncertainty and Validation Study

Aerosols are one of the major components that affects climate and air quality. Being able to measure global aerosol comprehensively has been a major goal for the last several decades. Now with the increasing number of sensors that are capable of retrieving aerosols on both geostationary orbit (GEO) and low-Earth orbit (LEO), getting a complete picture of global aerosol distribution is more achievable than ever. However, how to use these data with various temporal and spatial resolution synergistically is one of the

urgent questions that needs to be answered before combining products. Using a consistent Dark Target algorithm on three GEO sensors (two Advanced Baseline Imagers (ABI) on GOES-E and GOES-W and Advanced Himawari Imager (AHI) on Himawari-8) and three LEO sensors (Moderate resolution Imaging Spectrometers (MODIS) on Terra and Aqua and the Visible Near-Infrared Imaging (VIIRS) on Suomi-NPP), we evaluate six level 2 DT aerosol optical depth (AOD) products against Aerosol Robotic Network (AERONET) as well as Marine Aerosol Network (MAN) and investigated the similarity and differences among the products with a special focus on the two GEO and LEO common regions, namingly North America and East Asia. The error statistics of these products are generated against observing conditions with major uncertainty sources identified. Our results provide baseline evaluation results before synergy of DT aerosol products can be pursued.

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MS224

Simulate Extreme Wildfire with a Climate Model: Preliminary UQ Application and Challenges

Wildfires play an important role in the climate system via interactions with atmosphere, land, radiation, and biogeochemistry. Recent observations and model projections show a clear increasing trend of more extreme wildfires with climate change. Large wildfires can trigger pyrocumulonimbus (PyroCb) convection, an extreme thunderstorm. The stratospheric aerosol injected by large wildfires has been estimated to be similar to that from moderate volcanic eruptions. Although its importance is widely recognized, the fidelity of wildfire simulations remains relatively poor due to large uncertainties in the current global Earth system models and observational data. Here we built a new global multiscale simulation framework with the cutting-edge developments of climate modeling and observational data to provide the end-to-end testbed capabilities considering the highly uncertain aspects. We can simulate large (i.e., PyroCb) California wildfires with the observationally constrained emissions and surface forcings, convection-permitting scale dynamics, and interactive chemistry and aerosols. The off-the-shelf uncertainty quantification (UQ) method was applied to quantify the relative importance of main parameters. We found that plume injection height was the most important factor. The optimal parameter set improves the wildfire simulation quality. We will highlight the challenges in the current wildfire simulations with climate models and the needs for new UQ methods.

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MS225

Efficient Uncertainty Quantification of Digital Twins Using Neural Networks and Sequential Sampling

An important part of digital twinning is the construction of an accurate model of the physical system and the quantification of uncertainty in support of health monitoring and decision making. This talk will present a method to simultaneously construct a fast model of the underlying system and propagate uncertain input parameters to yield the desired statistics of the output quantities of interest. In particular, a novel extension to the efficient global optimization (EGO) algorithm is presented that uses neural networks (NNs) and sequential sampling to create a fast and accurate global approximation model of the underlying system. Given this approximation model, Monte Carlo simulation can be used to quickly compute the desired statistical information for the purpose of uncertainty quantification (UQ). The proposed EGO with NNs algorithm (or EGONN) models the system response as well as the spatial error of the system response prediction. By maximizing the prediction uncertainty model, a new sample point is found and appended to the current data set for training the system prediction model. Since the prediction is being updated in each sequential sampling cycle it allows for termination of the UQ process based on convergence of the summary statistics. The proposed method will be demonstrated through several numerical examples of aerospace systems using physics-based simulation data. Future research directions will be discussed.

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MS225

UQ-Based Digital Twinning for Structural Health Monitoring

The concept of a digital replica has evolved from the digital twin prototype (DTP) of 40 years ago i.e., a digital representation of a platform before it is manufactured to include the digital twin instance (DTI) i.e., the DT of an individual instance of a platform, after it is deployed. A DTI collects and processes sensor data to interrogate about a platform. Preliminary forms of this concept are often described as the integration of data analytics with the model-based prediction of a few, scalar, quantities of interest (QoIs). This talk however will question whether a few QoIs can always be identified to represent the critical state of a newly deployed physical platform to monitor its state in general, and its structural health in particular. Next, it will present a more robust approach for realizing a DTI for structural health monitoring that is based on adaptable, stochastic, low-dimensional but high-fidelity computational models. The approach features novel mathematical ideas for integrating model-form UQ with probabilistic reasoning, projection-based model order reduction, and machine learning. It constructs stochastic, physics-based computational models that self-adapt using information extracted from sensor data; operate in real time; and can be exploited to perform structural health monitoring. The lecture will demonstrate the potential of the proposed approach by illustrating it for a maintenance problem pertaining to a mockup fighter jet.

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MS225

A Tutorial on Uncertainty Quantification in Machine Learning for Health Prognostics

Over the past decade, many research studies have been undertaken to create and validate machine learning (ML) algorithms and methods for predicting the life of an engineered system/component based on data collected from the system/component. This tutorial will focus on quantifying and assessing ML models' predictive uncertainty in health prognostics applications. It will consist of three parts. The *first* part will be an overview of health prognostics and answer the question of why uncertainty quantification (UQ) of machine learning (ML) models is important. The *second* part will be a tutorial-style description of two state-of-the-art UQ methods: Gaussian process regression and neural network ensemble. The *third* part will demonstrate these UQ methods using an engineering case study on the life prediction of lithium-ion batteries at the early stage.

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MS225

An End-to-end Digital Twin Paradigm for Space missions: Fuel the Analytics

Digital Twins (DTs) promise a transformation in space exploration, with early adoption being key for competitiveness. Services like risk-informed decision-making are vital across the space system lifecycle, but the analytical and computational hooks have not been strategically framed for the space industry. Viable DTs for complex space systems must mirror lifecycle-evolving system needs. For example, during the design phase, generation and evaluation of the architecture trade space and functional allocation to physical form are fundamental. A DTs analytical framework must generate, assess, and optimize system architecture trades, while producing required compliance documentation. In the verification, validation, and test phase, a campaign is developed and executed to confidently ensure system robustness and reliability, predicting performance and identifying shortfalls. In the operations phase, incoming telemetry must be assimilated and mined to aid system health prognostics/diagnostics. System lifetime and science preservation are prevailing risks serviced continuously by the DT. Powering this scope requires a sophisticated analytics and computing infrastructure. The DT harnesses an agent that summons the requisite analytical/computing tooling, leveraging advanced techniques in UQ/ML/AI. This presentation explores essential DT analytics and their strategic orchestration in space systems.

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MS226

Estimation of Extreme Risk Measures with Neural Networks

We propose new parametrizations for neural networks in order to estimate extreme Value-at-Risk and Expected-Shortfall in heavy-tailed settings. All proposed neural network estimators feature a bias correction based on an extension of the usual second-order condition to an arbitrary order.The convergence rate of the uniform error between extreme log quantities and their neural network approximation is established. The finite sample performances of the neural network estimator are compared to other bias-reduced extreme-value competitors on both real and simulated data. It is shown that our method outperforms them in difficult heavy-tailed situations where other estimators almost all fail.

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MS226

Estimating Point Processes from Diffusion Excursions

Rare events are often modeled according to their arrival times through a point process interpretation. In this case, point processes have a natural interpretation with respect to a continuous process. We describe a point process construction that represents arrival time observations in terms of the state of a latent diffusion process based on Ito's excursion theory. In this framework, we relate the return time of diffusion in a continuous path space to new arrivals of the point process. These models arise in many disciplines, such as financial settings where actions in a market are determined by a hidden continuous price or in neuroscience where a latent stimulus generates spike trains. We describe computational methods for inferring and sampling from the point process derived from the diffusion process. Finally, we relate the excursion approach to existing interpretations with respect to extreme value theory.

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MS226

Botied: Multi-Objective Bayesian Optimization with Tied Multivariate Ranks

Many scientific and industrial applications require joint optimization of multiple, potentially competing objectives. Multi-objective Bayesian optimization (MOBO) is a sample-efficient framework for identifying Pareto-optimal solutions. We show a natural connection between non-dominated solutions and the highest multivariate rank, which coincides with the outermost level line of the joint cumulative distribution function (CDF). We propose the CDF indicator, a Pareto-compliant metric for evaluating the quality of approximate Pareto sets that complements the popular hypervolume indicator. At the heart of MOBO is the acquisition function, which determines the next candidate to evaluate by navigating the best compromises among the objectives. Multi-objective acquisition functions that rely on box decomposition of the objective space, such as the expected hypervolume improvement (EHVI) and entropy search, scale poorly to a large number of objectives. We propose an acquisition function, called BOTIED, based on the CDF indicator. BOTIED can be implemented efficiently with copulas, a statistical tool for modeling complex, high-dimensional distributions. We benchmark BOTIED against common acquisition functions, including EHVI and random scalarization (ParEGO), in a series of synthetic and real-data experiments. BOTIED performs on par with the baselines across datasets and metrics while being computationally efficient.

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MS226

Learning to Simulate Tail-Risk Scenarios

The estimation of loss distributions for dynamic portfolios requires the simulation of scenarios representing realistic joint dynamics of their components. Scalability to large or heterogeneous portfolios involving multiple asset classes is particularly challenging, as is the accurate representation of tail risk. We propose a novel data-driven approach for the simulation of realistic multi-asset scenarios with a particular focus on the accurate estimation of tail risk for a given class of static and dynamic portfolios selected by the user. By exploiting the joint elicitability property of Value-at-Risk (VaR) and Expected Shortfall (ES), we design a Generative Adversarial Network (GAN) architecture capable of learning to simulate price scenarios that preserve tail risk features for these benchmark trading strategies, leading to consistent estimators for their VaR and ES. We prove that the generator in our GAN architecture enjoys a universal approximation property under the criteria of tail risk measures. We also show that the bi-level optimization formulation between the generator and the discriminator is equivalent to a max-min game, leading to a more effective and practical formulation for training. We demonstrate the accuracy and scalability of our method via extensive experiments using synthetic and market data.

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MS228

Towards Multilevel Slice Sampling for Bayesian In-

verse Problems

Slice sampling is a Markov chain Monte Carlo method for drawing (approximately) random samples from a given posterior distribution, which is in general only known up to a normalizing constant. The method is based on sampling a new state on a slice, i.e., a level set of the target density function. Slice sampling is especially interesting because it is tuning-free and we always move to a new state which could result in a lower autocorrelation compared to Metropolis-Hastings, for example. However, to find such a new state can possibly require many evaluations of the target density and thus yield high computational costs. Therefore, in this talk we introduce the so-called delayed acceptance slice sampler. The idea behind this is that we exploit a cheap approximation to the target density for finding potential new states. We formulate certain properties, illustrate the advantage of the cost reduction in a Bayesian inverse problem and give a result, which shows, that the delayed acceptance slice sampler is theoretically more efficient than the delayed acceptance Metropolis-Hastings algorithm. Moreover, we present an approach for extending our two-level method into a multilevel framework.

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MS228

Multilevel Optimization-Based Sampling for Large-Scale Inverse Problems

We combine the multilevel Monte Carlo and the optimization-based samplers, including Randomized-and-Then-Optimize (RTO) and Implicit Sampling, to address the challenges that classical MCMC faces, and implements the samplers in computationally costly Bayesian inverse problems including an ODE model and a PDE problem. Simulations using the optimization-based samplers like RTO can be parallelized which allows us to develop efficient MCMC algorithms or self-normalizing estimators to solve the inverse problems. Multilevel Monte Carlo is proven to significantly reduce the computational cost of Monte Carlo simulation, which helps us further improve the RTO method. To adapt the multilevel method on the optimization-based samplers, we develop the complexity theorem for multilevel self-normalizing estimators. The corresponding numerical experiments produce good results on RTO method, showing a high effective sample ratio in the importance sampling scheme, and the variances of the self-normalizing estimators converge when discretization size decreases.

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MS228

Coupled Parameter-Data Dimension Reduction for Bayesian Inference

We introduce a novel approach to dimension reduction in Bayesian inverse problems. Traditionally, dimension reduction techniques have focused on either parameter or data spaces separately. However, choosing a low-dimensional informed parameter subspace influences which data subspace is informative and vice versa. Our method simultaneously reduces the dimensionality of both spaces by leveraging gradients of the forward model. It can be easily implemented in form of an alternating eigendecomposition algorithm. Moreover, our method allows for goal-oriented dimension reduction by prescribing a specific parameter or data subspace. We demonstrate its application in Bayesian optimal experimental design, where the goal-oriented data dimension reduction objective is related to maximising the expected information gain of the observation subspace.

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MS228

Inferring Functions with Uncertain Regularity

This work describes a Bayesian framework for reconstructing functions with uncertain regularity, i.e. roughness vs. smoothness. The regularity of functions carries crucial information in many inverse problem applications, e.g., in medical imaging for identifying malignant tissues or in the analysis of electroencephalogram for epileptic patients. We characterize the regularity of a function with its fractional differentiability. We propose a hierarchical Bayesian method which estimates a function and its regularity, simultaneously. In addition, we quantify the uncertainties in the estimates. Numerical results suggest that the proposed method is a reliable approach for estimating functions in different types of inverse problems. Furthermore, this is a robust method under various noise types, noise levels, and incomplete data.

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MS229

Continuous-Time Inference for Partially-Observed Markov Processes

Many natural and engineered systems can be modeled as Markov processes, but often, only a subset of states are directly observable. Hence, inferring the conditional probability that a system occupies a particular hidden state, given the partial observation, is a problem with broad application. In this talk, we discuss continuous-time formulations of the sum-product algorithm, a well-known discrete-time method for finding the hidden states' conditional probabilities, given a set of finite, discrete-time observations. We will primarily focus on the discrete-state setting where conditional probabilities can be written in terms of solutions to systems of ordinary differential equations. The continuous-time formulation allows for an explicit and efficient algorithm for finding the conditional probability of occupying any state. Finally, we will conclude by demonstrating the applicability of the algorithm to realistic biological systems and discussing future directions.

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MS229

Dynamical Closure in Complex Systems Using Quantum Mechanics

We present a data-driven scheme for learning closures of dynamical systems (i.e. parametrizations) based on the mathematical framework of quantum mechanics and Koopman operator theory. Given a system in which some components of the state are unknown, this method models the unresolved degrees of freedom as being in a time-dependent quantum-state, which determines their influence on the resolved variables. The quantum state is an operator on a space of observables and evolves over time under the action of the Koopman operator. The quantum state representing the unresolved degrees of freedom is updated at each timestep by the values of the resolved variables according to a quantum Bayes law. Moreover, kernel functions are utilized to allow the quantum Bayes law to be implemented numerically. We present applications of this methodology to the Lorenz 63 and multiscale Lorenz 96 systems, and show how this approach preserves important statistical and qualitative properties of the underlying chaotic systems.

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MS229

Variational Bayes vs Sample Continuation for UQ in Hierarchical Inference

Hierarchical Bayesian methods use a sequence of priors to constrain inference. The hyperparameters used encode the specific prior assumptions enforced. How robust are ensuing estimates to uncertainty in the hyperparameters? What is the functional relationship between assumptions and estimate? We study a path-tracing method for studying the sensitivity of estimates to uncertainty in the hyperparameters and compare variational inference methods and sample continuation methods for uncertainty quantification that leverage the continuous relationship between hyperparameters and posterior. By first drawing samples in a hyperparameter regime where the posterior is log convex, then continuously adjusting the hyperparameters towards the target problem, we can "continue" samples from a log-convex posterior to a highly non-convex target density. These methods allow a user to directly test the sensitivity of point estimates and confidence intervals to variability in prior assumptions.

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MS229

Exact Posterior Inference in Dynamic, Spatio-Temporal Stochastic Epidemic Models

We propose novel data-augmented Markov Chain Monte Carlo strategies to enable exact Bayesian inference under the stochastic susceptible-infected-removed model and its variants. Whether there is missing data in the trajectories due to only a partially informative glimpse of the underlying continuous-time process, or unknown labels in transmission types or direction, latent variables provide a powerful paradigm to bridge missing information to tractable Bayesian machinery. We show how to efficiently propose latent variables from surrogates that are carefully designed to closely resemble the SIR model yet admit simple forms for conditional sampling. This allows us to efficiently generate epidemics consistent with the observed data, and extends to non-Markovian settings as well as tasks such as simultaneous change-point detection under time-varying transmission and spatio-temporal smoothing. Our Markov chain Monte Carlo algorithm is shown to be uniformly ergodic, and we find that it mixes significantly faster than existing single-site samplers on several real and simulated data applications

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MS230

Certifiable Deep Importance Sampling for Rare-Event Simulation

Rare-event simulation techniques, such as importance sampling (IS), constitute powerful tools to speed up challenging estimation of rare catastrophic events. These techniques often leverage the knowledge and analysis on underlying system structures to endow desirable efficiency guarantees. However, black-box problems, especially those arising from recent safety-critical applications of AI-driven physical systems, can fundamentally undermine their efficiency guarantees and lead to dangerous under-estimation without diagnostically detected. We propose a framework called Deep Probabilistic Accelerated Evaluation (DeepPrAE) to design statistically guaranteed IS, by converting black-box samplers that are versatile but could lack guarantees, into one with what we call a relaxed efficiency certificate that allows accurate estimation of bounds on the rare-event probability. We present the theory of Deep-PrAE that combines the dominating point concept with rare-event set learning via deep neural network classifiers, and demonstrate its effectiveness in numerical examples including the safety-testing of intelligent driving algorithms.

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MS230

Conservative Assessments of Risk Probabilities Using Surrogates

We consider the problem of computing consistent and conservative estimators of exceedance probabilities of a one-dimensional, decisional quantity, described as the output of some black box model, using machine learning-based surrogates. This problem is key for design and monitor critical systems and study the structural safety of these systems. After a review of available approaches, we examine the possibility of obtaining deterministic bounds for calculations based on surrogates, and then describe how the estimator thus obtained can be guaranteed to be relevant to the true probability associated with the black box model. This work takes advantage of recent results based on non-asymptotic control of estimators, through concentration inequalities.

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MS230

Sensitivity-Informed Nonparametric Adaptive Conditional Sampling for Robust Reliability Analysis

Numerical models allow to simulate the behavior of complex systems, considering a set of deterministic input parameters. In this computer experiments framework, one may analyze the systems reliability by propagating input uncertainties through the model and estimating risk measures on the uncertain outputs obtained (e.g., rare event probabilities). This estimation is usually more difficult for highly nonlinear models and for very rare events. To overcome this challenge, a wide range of methods have been developed in the structural reliability community. Among them, adaptive sampling strategies (e.g., subset sampling) aim at breaking down a rare event into a nested sequence of conditional events (individually less rare). This mechanism eases considerably the estimation of rare event probabilities, however, it often relies on Markov Chain Monte Carlo sampling and offers limited guarantees. In this work, the new adaptive sampling strategy presented directly offers dedicated sensitivity information as a post-processing of the reliability analysis. Thanks to its independent sampling, a reliability-oriented sensitivity analysis is performed on each subset using sensitivity measures such as the target-HSIC (Hilbert Schmidt Independence Criterion). This additional sensitivity analysis is a simulation-free complementary tool, improving the understanding of a problem and making its resolution more robust.

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MS230

Decision Criteria for Risk Analysis in Presence of Two Levels of Input Uncertainty

Simulation plays a fundamental role in risk analysis of complex systems. In a probabilistic framework, i.e. when the feared events and imperfectly known characteristics of the system under consideration are modeled by random quantities, the demonstration of system safety is generally based on two distinct steps: estimating the probability of system failure (assumed to be associated with a rare event) and comparing it with safety standards or expert knowledge, in order to decide whether or not this value is sufficiently low. Although many efforts have been made to develop various efficient approximation or estimation techniques (possibly using advanced adaptive strategies based on surrogates) over the last few decades, few studies have really focused on the decision-making phase. The work to be presented therefore focuses on this second phase, and aims to propose decision criteria that can control, with high probability, the fact of designating as safe a system that would not be. In this context, particular attention will be paid to the case where uncertainties affecting the system parameters are imperfectly known, generating a double source of uncertainty which must be properly integrated for a correct risk analysis.

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MS231

A Generalization of the Circe Method for Quantify-

ing Input Model Uncertainty in Presence of Several Groups of Experiments

The semi-empirical nature of best-estimate models closing the balance equations of thermal-hydraulic (TH) system codes is well-known as a significant source of uncertainty for accuracy of output predictions. This uncertainty, called model uncertainty, is usually represented by multiplicative (log)-Gaussian variables whose estimation requires solving an inverse problem based on a set of adequately chosen real experiments. One method from the TH field, called CIRCE, addresses it. We present in the paper a generalization of this method to several groups of experiments each having their own properties, including different ranges for input conditions and different geometries. An individual (log-)Gaussian distribution is therefore estimated for each group in order to investigate whether the model uncertainty is homogeneous between the groups, or should depend on the group. To this end, a multi-group CIRCE is proposed where a variance parameter is estimated for each group jointly to a mean parameter common to all the groups to preserve the uniqueness of the best-estimate model. The ECME algorithm for Maximum Likelihood Estimation developed by Celeux, Grimaud & de Rocquigny (2010) is extended to the latter context, then applied to relevant demonstration cases. Finally, it is tested on a practical case to assess the uncertainty of critical mass flow assuming two groups due to the difference of geometry between the experimental setups.

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MS231

Bayesian Calibration and Metamodeling Applied to Thermal-Hydraulics Separate Effect Tests for Uncertainty Determination and Bias Correction

Nuclear power plant safety is typically assessed with thermal hydraulics system codes, which can model a large variety of accidental scenarios. Accidental transients typically include several physical phenomena. Each phenomenon is in turn estimated using closure models, whose parameters are informed from simpler Separate Effect Tests (SETs). The parameter nominal values and PDFs, previously determined by expert judgment, are now assessed by more robust alternatives like Bayesian calibration (BC). However, calibrating SETs results is challenging. First, SETs have several time-dependent outputs, which requires some base. Second, the code is generally slow and metamodels must be used with Markov Chain Monte Carlo techniques. Third, and most importantly, the code is biased, and model inadequacy must be accounted for during calibration and extrapolated to cases for which the output uncertainty has to be evaluated. In this presentation we illustrate the first two points on reflood experiments from the FEBA and RBHT facilities, which featured several time-dependent outputs, as well as code biases. RBHT will further illustrate how the model deficiency could be transferred to similar experiments Gaussian processes. Finally, using experiments on choke-flow, we present how hierarchical Bayesian calibration can solve the model deficiency transferability problem and why it is so important to do so.

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MS231

Using Outlier Detection Techniques for the Analysis of Thermal-Hydraulics Computer Experiments in Loca Studies

Nuclear safety assessments involve the study of transients that could occur in the reactor boiler in case of some accidental events such as loss of coolant accidents (LOCA). These transients are simulated using thermal-hydraulics codes which outputs are the physical quantities characterizing the state of the system throughout the transient. Most of the time, these outputs take the form of functional data e.g. a time-indexed series of scalar values. In a UQ context, these data are potentially highly informative as for the physical phenomena at stake during the transient, but require the use of specific statistical methods to be exploited. Among functional data analysis methods, we choose here to focus on those coming from the outlier detection field. Outliers are generally defined as observations which do not come from the same distribution as the rest of a data sample and thus should be discarded or treated separately. However, outlier detection methods can also be used to identify simulations showing unexpected, atypical or extreme behaviors amid a set of numerical experiments. We will illustrate the potential of functional outlier detection (FOD) techniques when applied to the examination of LOCA simulation outputs and expose the particular method we developed to study the peak cladding temperature (PCT) of fuel rods during such transients.

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MS231

Inverse Uncertainty Quantification Methods of Nuclear System Thermal-Hydraulics Codes

This presentation will provide a comparative discussion of the major aspects of the inverse uncertainty quantification (IUQ) methodologies that have been used on the physical models in system thermal-hydraulics codes. IUQ methods can be categorized by three main groups: frequentist, Bayesian, and empirical. They are sometimes also referred to as deterministic (optimization-based), probabilistic (sampling-based), and design-of-experiments (DoE, forward propagation-based), respectively. The frequentist IUQ methods consider that the parameters have fixed but unknown values. Consequently, IUQ is formulated as an optimization problem, more specifically, maximization of the likelihood to find the best-fit values. The Bayesian IUQ methods also assume that the parameters have true but unknown values, but always use probabilistic treatment of these parameters with uncertain distributions, because it is impossible to quantify the exact values given limited available information. The empirical IUQ methods are based on adjusting the parameters in a trial-and-error manner without a robust mathematical basis. We used eight metrics to evaluate an inverse UQ method, including solidity, complexity, accessibility, independence, flexibility, comprehensiveness, transparency, and tractability. Such comparative evaluation is intended to provide a good guidance for users to select a proper inverse UQ method based on the problem under investigation.

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MS232

Subordinated Gaussian Processes for Renewable Energy Studies

As the power grid moves to a more renewable future, energy sources from weather-driven phenomena such as solar, wind and hydroelectric power will form an increasingly large portion of generation. Although, in principle, limitless, the uncertainty and variability of these resources challenge current grid operation paradigms. Our research program focuses on quantifying and understanding this variability using modern space-time stochastic process models with particular focus on applications in distributed solar photovoltaic systems. We review some recent efforts from our group in developing randomly time-changed, or subordinated, Gaussian processes, and discuss space-time implementations and challenges on a highly nonstationary and non-Gaussian irradiance dataset.

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MS232

Neural Likelihood Surface Estimation for Computationally Intensive Or Intractable Spatial Models

Likelihood-based inference tends to be computationally intensive or wholly intractable for many common models in spatial statistics. Examples include Gaussian processes for large data sets and models for spatial extremes. Recent work has used neural networks to predict parameters in these models, circumventing the intractability of likelihood computations. Prediction, however, depends on the choice of a prior on the parameters and does not provide a straightforward means of frequentist uncertainty quantification. In this talk, I will demonstrate how to use tools from likelihood-free inference to learn the likelihood function of intractable spatial processes using convolutional neural networks. In cases where the exact likelihood is available, the method provides similar point estimation and uncertainty quantification performance as exact likelihood computations at a fraction of the computational cost. When the likelihood is unavailable, this method can learn the otherwise intractable likelihood function, providing inferences that are superior to existing approximations. The method is applicable to any spatial process on a grid from which fast forward simulations are available.

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MS233

Hoeffding Decomposition Revisited

The ability to uniquely decompose square-integrable functions of dependent random inputs into a sum of functions of every possible subset of variables is key in the field of sensitivity analysis. Many approaches have been proposed in the literature, that either approximate such a decomposition or rely on rather restrictive assumptions on the probabilistic structure of the inputs. However, such a decomposition is achievable under two reasonable assumptions:
• Non-perfect functional dependence between the inputs;
• Non-degenerate stochastic dependence structure; Under those assumptions, it is possible to show that the space of real-valued square-integrable functions admits a coalitional direct-sum decomposition. For the task of variance decomposition, it leads to the definition of novel sensitivity indices, which generalize the well-known Sobol' indices.

Furthermore, this result allows for an intuitive definition of interaction and dependence effects. This talk is dedicated to presenting this result, discussing its implications, and highlighting the challenges to come for a practical implementation.

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MS233

Hsic Sensitivity Analysis for Discrete Variables

In this talk, we explore the possibility of performing sensitivity analysis using Hilbert Schmidt Independence Criteria (HSIC) [1] when dealing with categorical (i.e., qualitative) covariables and/or variables of interest. In practice, the main challenge consists in defining proper and informative covariance kernels between categorical values, as well as identifying their optimal parameterization. We consider here a kernel based on the projection of the categorical variables levels onto d-dimensional continuous latent variables [2], and analyze the possibility of identifying the optimal projection coordinates so as to maximize the HSIC indices values. A complementary analysis is provided on how to avoid identifying spurious dependencies between variables when dealing with finite data sets. [1] Gretton, Arthur, et al. (2007). [2] Zhang, Yichi, et al. "(2020).

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MS233

Optimal Variance in the Chatterjee Method Estimation of Sobol Index

Chatterjee's method provides arguably the simplest way to estimate first order Sobol indices, as the empirical auto-correlation of the response variable obtained upon reordering the data by increasing values of the inputs. This idea can be extended to higher lags of auto-correlation, thus providing several competing estimators of the same parameter. We show that these estimators can be combined in a simple manner to achieve the theoretical variance efficiency bound asymptotically.

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MS233

Sobolev Space, Tchebytchev Interpolation and Sensitivity Analysis

In this talk, our aim is to promote the use of the so-called Poincar basis for Uncertainty Quantification (UQ), particularly when derivative information is available. Formed by the eigenfunctions associated with Poincar inequalities, the Poincar basis is the unique orthonormal basis of the one-dimensional Sobolev space $H^1(\mu)$ that remains an orthogonal basis of $L^2(\mu)$ after differentiation. We will explore two applications of the Poincar basis within UQ. Firstly, in the context of global sensitivity analysis, the Poincar basis proves invaluable for calculating Sobol' indices in a manner analogous to polynomial chaos expansions (PCE). It seamlessly accommodates derivative information and, notably, surpasses PCE in identifying inactive variables while making efficient use of computational resources. Secondly, the Poincar basis finds application in estimating integrals using quadrature formulas, specifically when the integrand belongs to $H^1(\mu)$. This problem can be conceptualized as a kernel quadrature problem, wherein $H^1(\mu)$ serves as a Reproducing Kernel Hilbert Space (RKHS). To address this challenge, we leverage the fact that the Poincar basis forms a Tchebytchev system.

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MS234

Decision-making Under Deep and Irreducible Un-

certainty with Implications for Climate Adaptation

Climate adaptation, whether low regrets or transformative, often hinges on global climate or earth system model simulations. However, gaps in our understanding of human behavior and socioeconomic systems, the physics and biogeochemistry of the earth systems, as well as internal or natural variability resulting from nonlinear dynamics and bounds to predictability, translate to what has been called deep and irreducible uncertainty in projections. Risk-informed decisions regarding the design and operations of lifeline systems, critical infrastructures, and key resources, usually depend on probabilistic characterizations of climate and weather changes and extremes and where possible, reduction of the uncertainties. Deep uncertainty refers to situations where such characterizations are not possible, while irreducible uncertainty arises from limits to predictability. Climate adaptation decisions are often further complicated by the need to inform decisions at high resolutions in space and time, which exacerbates the relative dominance of irreducible and deep uncertainties at decadal and century scales respectively. This presentation discusses prior and ongoing work to address these challenges. While the solutions range from physics-constrained Bayesian uncertainty characterizations, Bayesian Deep Learning, information-theoretic characterizations of nonlinear dynamical behavior, network-based uncertainty propagation, and carefully designed risk frameworks, open challenges remain.

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MS234

Simulation-based Slab Burner Analysis under Uncertainty: A Framework for Analyzing and Combining Uncertainties from Multiple Sub-models and Sources

In this talk, we discuss an uncertainty quantification framework for a simulation-based analysis of a hybrid rocket 2D slab burner. The output quantities of interest include the regression rate of the fuel, the heat flux at the fuel surface, and field quantities such as temperature. Creating an optimum model of a hybrid rocket motor is challenging because of the present multiscale turbulent combustion physics, which require detailed physics-based models for the atomization and generation of droplets, the chemical kinetics, the turbulent combustion source energy, and the flow solver. A further problem is that for these sub-models: a) it is not known a priori what some parameters should be (e.g., latent heat of vaporization of the fuel) and b) the inputs to most sub-models are also uncertain (e.g., inlet conditions, chemistry). In this talk, we will present appropriate strategies to overcome these challenges (variance-based global sensitivity to select a subset of reactions based on chemical kinetics, a neural network for tabulation of the source energy, surrogates for expensive simulations, and Bayesian calibration for unknown parameters) and our current work of coupling each of these processes with the main simulation of the slab burner.

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MS234

Deep Generative Models with Latent Representation for High-Fidelity 3D Digital Materials

The rapid advancement of additive manufacturing technologies enables a pixelated or voxelated structure consisting of multiple materials in 2D or 3D, respectively, called digital materials. It maximizes design flexibility without constraints in geometry and material, realizing unprecedented physical properties and functionalities that cannot be realized by conventional manufacturing processes. However, the enormous design space of digital materials has become a significant challenge for maximizing the availability of digital materials. In this study, we developed a novel deep generative model with discrete representations of the latent space for designing digital materials. The proposed model, inspired by the discrete nature of digital materials, retains reconstruction and prediction accuracies with one-third of the data usage compared to the conventional generative model. The physical insight of discrete representations of latent space is rigorously interpreted, proving that certain discrete representations are strongly related to the mechanical behavior of digital materials, such as auxeticity. It was also confirmed that the proposed model is an excellent tool for generating functionally graded structures as well as the unseen auxetic structures.

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MS234

Optimal Control through semi-Gaussian Bayesian Update

This study proposes a semi-Gaussian Bayesian update framework for optimal control and data assimilation. In particular, the study focuses on an ensemble-based approach for such goals. The framework will provide insights into the meaning of inflation and sampling error correction (or localization) that are commonly used in the ensemble-based Bayesian update methods, such as ensemble transform or adjustment Kalman filters. The study further provides a strategy for designing a new sampling error correction instead of the distance-based ad hoc approach for the error correction.

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MS235

Surrogate Modeling and Inverse Estimation for Design, Optimization, and Control of the Sintering Process

We are interested in inverse problems arising in the control of the sintering process which are critical for applications such as 3D printing and fabrication of electronics. High-fidelity simulations of the sintering process involve non-

linear material models like viscoelasticity or viscoplasticity coupled with thermal and electrical phenomena. These simulations are typically computationally expensive and are thus often difficult to use for performing design, optimization, process control, and inverse estimation. To expedite the inverse estimation of sintering process parameters or material properties, we present a combination of online-efficient model order reduction technique and data assimilation. Firstly, we employ Proper Orthogonal Decomposition in conjunction with Gaussian Process Regression (POD-GPR) to construct a non-intrusive and online efficient surrogate model. Secondly, we use the Ensemble Kalman Inversion (EnKI) technique for performing inverse estimation given that it is parallelizable and does not require expensive derivative computations. In particular, we use a modified EnKI method based on an estimate of the model bias to mitigate an approximation error that arises upon using the surrogate model. Finally, we investigate the performance of the proposed method on a coupled nonlinear macroscopic sintering model in accelerating the inverse estimation of hard-to-measure material properties such as viscosity.

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MS235

A Framework for Developing Stable Spatio-Temporal Emulators with Deep Learning

Deep neural networks (DNN) have shown promise in building models that can auto-regressively emulate the spatio-temporal evolution of nonlinear dynamical systems, even for those as complex as the global weather system. Such emulators, which are fast during inference, have wide-ranging applications, including data assimilation, uncertainty quantification, and inverse problems. However, the current DNN-based emulators, while accurate in short terms, are unstable in long terms, significantly limiting their usefulness. Here, we first show, using a hierarchy of test cases and DNN architecture, that spectral bias, is the case of these instabilities, as it prevents the DNNs from learning the small scales. The errors in the small scales grow over time to large scales due to nonlinearities, leading to instabilities (blow-ups, unphysical drifts). We propose a new architecture, with regularized loss functions and better time integration schemes, that can reduce the spectral bias and suppress the error growth, producing stable simulations. We demonstrate the effectiveness of the new architecture across a hierarchy of systems, from the chaotic Kuramoto-Savishinky equation to global weather. We also show how the eigenanalysis of linearized DNNs provides insight into the stability properties of an architecture.

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MS235

Aerodynamics Predictions with Confidence Intervals Using Autoencoders

A convolutional autoencoder is trained to reproduce the aerodynamic characteristics of wing sections. The formulation is based on an adaptive training database that minimize the data required while preserving the accuracy of the solutions. The autoencoder uses aggressive compression (small latent dimension) to mimic the independent variables used to define the database; the latent space is interpolated using Radial Basis Functions with a cubic kernel to generate synthetic flow fields on unseen airfoils. The accuracy of the results and the interpretation of the latent space are based on comparisons with simulations. A protocol for quantifying the confidence in the autoencoder predictions is developed. The approach is based on a query-by-committee ensemble analysis and enables to identify the relative importance of the data and the auto encode hyperparameters.

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MS235

High-Dimensional Applications of Ensemble-Based Data Assimilation in Geosciences

In geoscientific data assimilation applications, like for state estimation, forecasting, or parameter estimation in the atmosphere and ocean, complex high-dimensional models are used on supercomputers. Ensemble simulations provide uncertainty estimates, but increase the computing costs beyond single model runs. In addition, the model nonlinearity induces challenges because common methods like ensemble Kalman filters and variational methods, which typically minimize a quadratic cost function, base on Gaussian distributions, and hence imply linearity. This presentation will discuss the computational, algorithmic, and practical challenges in these applications and will further consider the relevance of the model with examples from ocean and ocean-ecosystem models.

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MS237

Reduced-Order Modeling for Parametric Dynamical Systems from Frequency-Domain Measurements: Addressing the Case of Multiple Parameters in Interpolatory Loewner Matrix Approaches

Reduced-order modeling is an effective approach used to simplify complex dynamical models while maintaining accuracy and reducing computational requirements. Traditionally, reduced-order models rely on the availability of state-space realizations that are sometimes unavailable in practice. Non-intrusive data-driven methods offer an alternative by constructing reduced-order models directly from data, bypassing the need for accessing an explicit realization. Among these methods, the Loewner framework by Mayo and Antoulas '07 provides a viable and effective way to construct reduced-order models from frequency response data. Its extension in the work by Antoulas, Lefteriu, and Ionita '12 showed how to generalize the interpolation scheme for fitting parametric models. There, it was explained how to construct realizations for bivariate rational functions, corresponding to the transfer functions of the fitted models (depending on one parameter only). In the current work, we provide extensions for such realizations that can cope with a general number of parameters. The dimension of the fitted models scale with the sum of the number of data points (in each dimension), and not with their product. Additionally, the construction of a quasi-Loewner matrix is required in the first steps of the method. We show that this matrix can be written as the solution of a generalized Sylvester equation, or of p+1 coupled standard Sylvester equations (with 2 terms each), in the case of p parameters.

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MS237

Compressed Kernel-Based Machine Learning Surrogates for the Uncertainty Quantification of Electronic Systems in the Frequency Domain

Uncertainty quantification (UQ) is of paramount importance in the design of modern electronics, as process variations and fabrication tolerances play a significant role in limiting electrical performance. Over the last two decades, polynomial chaos expansion (PCE) emerged as a powerful tool overcoming the inherent limitations of Monte Carlo in the number of samples required. On the other hand, machine learning surrogates are increasingly explored in the context of UQ. Nonparametric kernel-based methods, such as least-square support-vector machine (LS-SVM) and Gaussian process regression (GPR), showed promising performance in scaling to higher dimensions, while keeping the training cost within feasible limits. GPR uses a Bayesian setting that allows associating confidence levels to model predictions. In this talk, we focus on three aspects of kernel-based methods applied to UQ: 1) we introduce special kernels that allow drawing an equivalence between the PCE and LS-SVM, based on which the former can be constructed using the more convenient and parsimonious formulation of the latter; 2) we develop more accurate and conservative estimates of the GPR confidence, and we extend it to UQ measures; 3) we introduce principal component analysis (PCA) to handle large and complex-valued output spaces referring to multiple frequency points. The full training dataset is compressed to a smaller dataset associated to the principal components, on which the training is efficiently performed.

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MS237

Fourier Transform Based Surrogate Modelling for High-dimensional Electric Machine Key Performance Indicators

Electric machine production is prone to numerous uncertainty sources that can cause noticeable deviations from key performance indicators (KPIs) corresponding to the nominal design. Exemplarily, stochastic design variations can introduce undesirable harmonic components in the torque, thus negatively impacting performance. Therefore, uncertainty quantification (UQ) for electric machine designs and KPIs is crucial. UQ studies for electric machines can be computationally intensive due to model complexity and resource requirements. To alleviate the computational burden, cost-effective surrogate models often replace expensive machine models. One such surrogate modelling approach is the use of machine learning (ML) models trained on available design data. A bottleneck here is the challenges encountered when surrogate models are called to approximate high-dimensional KPIs, e.g., torque over rotor angle. In such cases, dimension reduction techniques can be employed to reduce the output space prior to the surrogate modelling task. In this work, we take advantage of the specific waveform characteristics of high-dimensional electric machine KPIs and employ the Fourier transform to reduce their dimensionality, while still preserving essential physical information. Subsequently, surrogate models for the reduced Fourier coefficients are developed. This approach is compared against standard dimension reduction techniques (e.g., PCA, POD), showing distinct advantages.

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MS237

Complex-Valued Gaussian Process-Based Approximation of Frequency Response Functions

This work focuses on approximating a complex-valued function from data using Gaussian Processes (GPs) or kernel-based methods. We place special emphasis on frequency response functions associated to partial differential equations. While GPs are becoming more popular in this context, standard kernels or covariances often underperform. We introduce a new interpolation method, which relies on a dedicated choice of both covariance and pseudo-covariance function. Furthermore, we enhance the method by combining the GP interpolant with a low-order rational function, the order of which is adaptively selected based on a novel model selection criterion. The low-order function turns out to be essential to capture strong dynamic responses of underdamped systems. We further discuss the quantification of uncertainty within the GP framework. From the kernel perspective, we introduce new reproducing kernel Hilbert spaces for complex-valued functions, and we frame the problem of complex-valued interpolation using a kernel pair as a minimum norm interpolation problem within these spaces. Numerical results from various fields, such as electromagnetics and acoustics, demonstrate the method's performance. We also compare it to existing rational approximation methods to highlight its effectiveness.

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MS238

Approximate Bayesian Reinforcement Learning

Model-free algorithms are used for control and optimization of complex (non-physical) systems. Reinforcement learning is a widely used model-free approach that has seen success in optimization of control applications and beyond. State and parameter estimation is a critical aspect of reinforcement learning in defining a model. While often described deterministically, some reinforcement learning algorithms can already account for a stochastic model through probability distributions often simplified to its first two moments, mean and variance. This paper describes reinforcement learning as an inverse problem through a Bayesian framework of conditional expectations for any stochastic model of uncertain parameters. From that, a general formulation of the Kalman Filter is presented for the estimation of states and parameters of the system. The derived operators are approximated by polynomial expansions, that can represent higher moments of the probability distribution. For practical implementation, the generalized Kalman Filter based Reinforcement Learning algorithm is applied to the classical control benchmark of the inverse pendulum.

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MS238

Non-Intrusive Operator Inference for Soft Continuum Robot Arm

The predictive modelling of soft continuum arm behaviour under quasi-static/dynamic conditions is often based on merging physics-based finite element (FE) models with experimental data. To deduce the underlying model parameters from observed data, one has to solve the corresponding high-dimensional inverse problem. In this paper we pose the parameter estimation problem in a probabilistic setting seen from a Bayesian point of view. The unknown model parameters are modelled as uncertain by use of the prior experts information. Observations on the displacement field are fused into this description to obtain the posterior. However, estimation of the likelihood function requires propagation of the parameter prior through the FE model. To enable online estimation, as is necessary for practical application in clinical setting, we pose the inference problem in a sequential manner. Although computationally efficient, this approach requires the cumbersome restarting of the FEM model at each increment. To address this problem we develop a hierarchical generalized Kalman filter approach that can be used for nonlinear problems and non-Gaussian parameter description. A master filter is responsible for the parameter estimation given observation data, whereas a slave filter is responsible for the estimation of the material state prediction given updated parameter. The novel approach is studied on a simple example of one soft segment exposed to different quasi-static loading conditions.

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MS238

Self-Organized Neural Networks

The discretization of parametric partial or ordinary differential equations describing complex physical phenomena leads to high-dimensional problems, the solution of which requires a massive computational effort. To address this challenge, the development of low-cost surrogates in a data driven manner is the main focus of this talk. To incorporate prior knowledge as well as measurement uncertainties in the traditional neural networks, an efficient sparse Bayesian training algorithm is introduced. By fine tuning specially designed priors the proposed scheme automatically determines relevant neural connections and adapts accordingly in contrast to the classical gradient-like solution. Due to its flexibility, the new scheme is less prone to overfitting, and hence can be used to approximate both forward and inverse maps by use of a smaller data set. The optimal choice of the measurement data then can be easily achieved by maximizing the information gain. In this talk the new type of learning will be showcased on a high-dimensional stochastic partial differential equation describing the nonlinear mechanics problem, as well as on the Lorenz type of time dependent problem including uncertainties.

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MS239

Domain Decomposition for Large Neural Networks Describing Battery Mechanical Response

One of the main challenges in electrified automotive vehicles is to ensure mechanical safety of battery packs made of thousands of Li-Ion battery cells. These cells are subjected to large deformations which can cause chemical instability. Therefore, one of the main challenges in designing battery cells is to predict their mechanical behavior, while including possible variations in design, material properties and boundary conditions. By including the probabilistic description of the relevant parameters, the highly nonlinear partial differential equations describing the problem become stochastic, and thus high dimensional. We design a novel surrogate model that consists of a domain decomposition method combined with deep learning. The idea is to partition domain into the linear and nonlinear regions, calculated in parallel. The method is based on the alternative minimization approach that inherits the objective functions from a classical or physics-inspired machine learning setting. The main challenge is the nonlinearity of the problem as well as the number of parameters describing the network. For this purpose we will present the novel training approach that takes linearization of the physics-based constraints and the inherent reduction of the number of parameters into account through the prospective sensitivity analysis. The numerical convergence of the method will be showcased on few simple analytical examples, as well as simplified mechanical model of the battery cell.

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MS239

Covariance Estimation Using H-statistics in Monte Carlo and Multilevel Monte Carlo Methods

Efficient estimation of covariance of probabilistic responses is crucial in Bayesian inverse problems like Kalman filtering-type data assimilation and uncertainty analysis tasks such as variance- and covariance-based sensitivity analysis. Traditional methods like vanilla Monte Carlo prove impractical due to slow convergence and high computational demands. The multilevel Monte Carlo method (MLMC) addresses these challenges by distributing the sampling strategy across fidelity levels. While initially designed for mean determination, extensions to MLMC, including covariance estimation, have been proposed. This study introduces a novel MLMC method for unbiased covariance determination using h-statistics. The procedure's advantage lies in the unbiased construction of the estimator's mean square error in a closed form, contrasting with the conventional MLMC estimator based on biased mean square errors defined solely on upper bounds. Finally, the numerical results of the algorithm are demonstrated on a simple 1D stochastic elliptic PDE such as Poisson's model.

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MT1

Principles of Data Assimilation and Sequential Inference

Data Assimilation lies at the heart of many important geophysical applications such as numerical weather prediction, and is increasingly being used for uncertainty quantification and real time prediction in many time-dependent systems. It allows for the seamless integration of noisy data and imperfect models in real time in order to provide estimates of system states or parameters, along with their respective uncertainties. However, this is typically non-trivial to implement in practice in the case of non-linear models and/or intractable and computationally expensive likelihood functions or observation operators. In this tutorial, we will start with the underlying principles of various data assimilation methods (including variational and sequential Bayesian methods), before discussing their interrelations, Monte Carlo based extensions, and modern challenges. A variety of modern data assimilation methods designed to alleviate computational challenges related to

high dimensional inference and non-Gaussianity will also be discussed.

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MT2

Multi-Fidelity Statistical Estimation and Surrogate Modeling

Accurately quantifying uncertainty in the predictions of high-fidelity numerical models can require an intractable amount of computational resources even when using supercomputers because even a single simulation may take over O(10000) CPU hours. While, cheaper lower-fidelity models, e.g. based on coarse numerical meshes, can be used to facilitate more extensive exploration of model uncertainties, they introduce a bias into estimates of uncertainty that must be accounted for. Consequently, this tutorial will introduce multi-fidelity methods that combine a limited number of high-fidelity simulations, used to minimize bias, with larger amounts of lower fidelity simulations used to reduce computational cost. The first half of the tutorial will review Monte Carlo (MC)-based multi-fidelity methods for estimating model statistics such as mean and variance and provide insight on the relationships between popular methods including multi-level MC, multi-fidelity MC, approximate control variates and multi-level best linear unbiased estimators. The second half of the tutorial will review methods for constructing surrogates from multi-fidelity data. Focus will primarily be given to multi-fidelity Gaussian processes and polynomial approximations, but the talk will conclude with more recent advances and open challenges. Each topic will be complemented with numerical examples implemented in PyApprox https://github.com/sandialabs/pyapprox.

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MT3

Rare Event Estimation with PDE-Based Models

TBD

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MT4

Generative Machine Learning Models for Likelihood Estimation

We will survey the use of machine learning generative models for likelihood estimation. Generative models are trained on data and then used to generate novel samples from the same distribution as the training data. In the field of machine learning, generative models are best known for creating human-like novel images and text. Generative models are also useful in uncertainty quantification. Certain generative models consist of both the forward generative function and a backward function that computes the likelihood of a given point. We will first provide an overview and comparison of the most popular approaches: generative adversarial networks (GAN), variational auto encoders (VAE) and normalizing flows. We will then go into more depth on normalizing flows including the mathematical foundations, as well as practical considerations for implementing UQ approaches with generative models. Finally, we will demonstrate example applications in the analysis of observational data from Mars and from neutron stars.

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MT5

PyDMD - Dynamic Mode Decomposition with Python

PyDMD is a Python package designed for Dynamic Mode Decomposition (DMD), a data-driven method used for analyzing and extracting spatiotemporal coherent structures from time-varying datasets. The package implements many extensions to handle noisy data, to impose structure on the learned operators, and to provide uncertainty estimates. PyDMD has a comprehensive and user-friendly interface, making it a valuable tool for researchers, engineers, and data scientists working in various fields. After this mini tutorial, participants will be able to use all the main functionalities of the package, how to exploit Bagging-Optimized Dynamic Mode Decomposition for uncertainty quantification, and to develop new DMD classes.

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MT5

PydDMD - Dynamic Mode Decomposition with Python

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MT5

PyDMD - Dynamic Mode Decomposition with

Python

PyDMD is a Python package designed for Dynamic Mode Decomposition (DMD), a data-driven method used for analyzing and extracting spatiotemporal coherent structures from time-varying datasets. The package implements many extensions to handle noisy data, to impose structure on the learned operators, and to provide uncertainty estimates. PyDMD has a comprehensive and user-friendly interface, making it a valuable tool for researchers, engineers, and data scientists working in various fields. After this mini tutorial, participants will be able to use all the main functionalities of the package, how to exploit Bagging-Optimized Dynamic Mode Decomposition for uncertainty quantification, and to develop new DMD classes.

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PP1

Survival Analysis on Papillary Thyroid Cancer Through Cox Proportional Hazard Model

Cancer disease is the second leading course of death in our society and it accounts every sixth death. Thus, the survivorship of cancer patients plays an important role among medical professional and many research studies have been done based on identifying the risk factors and their contribution to the patients survival. Thyroid cancer is one of the important cancers that has been increasing in the United States. There are four main types of Thyroid cancer: Papillary, Follicular, Anaplastic and Medullary. Papillary Thyroid Cancer, PTC is the most common Thyroid cancer type accounting for eight out of ten Thyroid cancer patients which leads our research focus on the PTC. The main objective of this study is to develop a semi-parametric Cox Proportional Hazards model which is commonly used in medical studies, to investigate the association between the survival time of PTC patients and five risk factors: Age, Sex, Malignant tumor size, Race and Stage of the cancer. Our final Cox-PH model is statistically significant with three individual risk factors and three two-way interaction terms which specifies how these risk factors influence the rate of death (hazard rate) at a particular time point by satisfying all the assumptions. Then we ranked all the individuals and their interactions based on hazard ratio to identify the most contributing individual risk factors and two-way interactions.

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PP1

Black-Box Constrained Optimization for Stochastic Simulators Using Multi-Fidelity Strategies

Many real-world systems in engineering and physics are modeled by complex simulators that might be parameterized by a high-dimensional random variable. Some notable examples include particle physics, fluid mechanics, molecular dynamics, protein folding, cosmology, material sciences, etc. Frequently, the simulators are black-box and computationally expensive (e.g., legacy solvers), making the task of optimization/inference challenging, specifically in high dimensions. The task can be further complicated with the inclusion of constraints. One can efficiently perform optimization only by utilizing the gradient with respect to the parameters, but these gradients are unavailable. In response to these challenges, we introduce the algorithm Scout-Nd (Stochastic Constrained Optimization for N dimensions) to tackle the issues mentioned earlier by efficiently estimating the gradient, thus enabling gradient-based optimization of simulator parameters. We employ methods to reduce the noise of the gradient estimator, and utilize multi-fidelity schemes to further reduce computational effort. We demonstrate on classical benchmark problems that our method performs better than the chosen baselines in terms of the quality of optimum and number of functional calls. We then present the results of a realistic use case involving a physics-based simulator.

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PP1

Topology Optimization for Denture Reinforcement

We develop a computational method to enhance the strength and durability of dental prostheses, by optimizing the reinforcement (E-glass material). Our research primarily focuses on the optimization of denture reinforcement. The objective for optimization is to minimize deformation by identifying specific areas within the prosthesis which could be implemented by modern multi-material three-dimensional printers. We apply our method to a three-dimensional removable lower jaw dental prosthesis to minimize compliance and reduce the risk of dental reinforcement fractures during clinical usage. To achieve this, we compare a non-reinforced denture (a material) and a reinforced denture (two materials). Our findings reveal that the reinforced denture has less maximum deformation and additionally, node-based displacement distribution indicates that the average displacement distribution is better in the reinforced denture.

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PP1

Conformal Object Detection

Object Detection is one of the most applicable prediction tasks in industrial cases. In the past years, plenty of models have been proposed, with significant structural and performance improvements. However, by definition of the task and by the approach taken to construct neural networks for this task, object detection models are very subject to uncertainty and instability. In this work, we adapt multiple approaches of statistical certification to object detection and propose several definitions of errors, that lead to different types and levels of guarantees.

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PP1

Advanced Sensitivity Analysis of the Impact of Precipitation Characteristics on RainfallRunoff Model Parameters

In the urban drainage system design and management, stormwater models play a strategic role. Recognizing and comprehending the inherent uncertainties within these models, as well as the implications on the resultant outputs, is paramount to ensure that ensuing decisions are underpinned by dependable data. Calibration of these models, coupled with a thorough sensitivity analysis, is essential to quantify their effectiveness in reproducing confidently a catchment area. Presently, hydrodynamic models are predominantly utilised for hydrograph simulation. Owing to the number of parameters that need to be tuned, challenges may arise during the calibration phase. To address this, sensitivity analysis (SA) is employed to minimise the number of parameters that need calibration. Many SA studies, however, often overlook the influence of event precipitation characteristics on the catchment outflow hydrograph. In this study, the Morris method was used to investigate the effect of 10 parameters on the discharge of a physically based rainfallrunoff model, accounting for the influence of rainfall depth on parameters significance. Results indicate that rainfall depth significantly affects sensitivity factors. Furthermore, once calibrated, the rainfall/runoff model demonstrated high predictive accuracy and the model outputs aligned closely with the measured data.

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PP1

Regularized Sampling of Fractional Gaussian Processes on R^d

In many applications of inverse problems, we face the problem of estimating continuous quantities from indirect measurements. In addition, we must quantify uncertainties in such an estimate. The infinite-dimensional Bayesian approach is a promising method for estimating continuous quantities in inverse problems. A key component for infinite-dimensional Bayesian inverse problems is to identify an appropriate prior distribution for the unknown continuous functions. The Whittle-Matern priors are a popular choice for such unknowns. However, incorporating spatial inhomogeneity, anisotropy, and local irregularities into such priors is challenging. We present an infinite dimensional prior for Bayesian inverse problems which incorporate spatial inhomogeneity, anisotropy, and local irregularities. To construct our priors we use the theory of elliptic pseudo-differential operators. We present samples of such prior, examine the regularizing effect of the inhomogeneity, and compare numerical results with the standard fractional Gaussian processes. This work has potential applications in many inverse problems with local inhomogeneity, e.g. in X-ray computed tomography, and fault detection in industrial applications.

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PP1

Computer Model Calibration for Large-Scale Spatially Distributed Counts

The Interstellar Boundary Explorer satellite (IBEX) was launched by NASA in 2008 and collects data that can help reveal the structure of the heliosphere, the bound-

ary between our solar system and interstellar space. In particular, IBEX detects energetic neutral atoms (ENAs) coming from the heliosphere. Space science theorists have developed a variety of competing models for ENA generation and propagation, and they want to use IBEX data to evaluate the relative strength of evidence for different models. This problem fits naturally within the framework of statistical computer model calibration. However, this problem also comes with some unique challenges, such as non-continuous data, limited but data-intense computer model runs and field measurements, nonstationarity of the response surface, and spatially correlated observations. We present a framework for model calibration that builds upon the canonical Kennedy and O'Hagan approach and incorporates scaled Vecchia-approximated Gaussian processes.

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PP1

Butterfly-Accelerated Gaussian Random Fields on Manifolds

Gaussian random fields are a class of stochastic process models which are widely used in spatial statistics and Bayesian inverse problems. However, the covariance matrix that defines the distribution of any finite set of observations is generally dense, which poses a computational challenge for large sample sizes. For stationary covariance functions in the plane, there exist several methods which express the random field as a superposition of Fourier modes, and use the fast Fourier transform (FFT) to accelerate computations. We propose a generalization of these methods for Gaussian random fields on manifolds. We express the random field in terms of eigenfunctions of the Laplace-Beltrami operator, and use a butterfly factorization - an algebraic generalization of the FFT - to accelerate computations. We demonstrate the performance of our method on triangle meshes discretized with finite elements, and discuss its application as a prior in Bayesian inverse scattering problems.

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PP1

Stochastic Differential Equations for Performance Analysis of Wireless Communication Systems

This paper addresses the challenge of characterizing the time-varying nature of fading channels. The current time invariant models often fall short in capturing and tracking these dynamic characteristics. To overcome this limitation, we ex- plore the use of stochastic differential equations (SDEs) to model signal envelope variations, considering scenarios involving Rayleigh, Rice, and Hoyt distributions. Furthermore, it is of practical interest to study the performance of channels mod- eled by SDEs. The outage probability (OP) has been the most commonly used performance measure. However, it does not provide enough information in specific communication system applications. In this work, we investigate a more general metric, the fade duration, representing the time during which the signal remains below a specified threshold within the interval [0 T]. Employing various approaches, including Monte Carlo (MC) and Kolmogorov Backward Equation (KBE), we estimate the complementary cumulative distribution function (CCDF) of the fade duration in the Rayleigh case, and analyze the impact of system parameters on its behavior. Finally, we leverage importance sampling (IS), a known variance reduction technique, to efficiently estimate the tail of the CCDF. Keywords: Fading channels, stochastic differential equations, fade duration, Monte Carlo, Kolmogorov Backward Equation, Importance sampling.

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PP1

A Double Polya-Gamma Data Augmentation

Scheme for a Hierarchical Negative Binomial - Binomial Data Model

We develop a double Polya-Gamma data augmentation scheme for posterior sampling from a Bayesian hierarchical model of total and categorical count data. The scheme applies to a Negative Binomial - Binomial (NBB) hierarchical regression model with logit links and normal priors on regression coefficients. The approach is shown to be very efficient and in most cases out-performs the Stan program. We apply the hierarchical modeling framework and the Pya-Gamma data augmentation scheme to human mitochondrial DNA data.

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PP1

Advanced Orthogonal Learning-Based Self-Adaptive Algorithms with Archives for Real-Parameter Optimization.

This article presents a set of strategies to enhance the Artificial Electric Field Algorithm (AEFA). These strategies encompass an orthogonal array-based initialization for improved population generation, an archive-based self-adaptive learning approach that categorizes the population into ordinary and extraordinary sub-populations, each employing distinct learning mechanisms, a mutation strategy to enhance the extraordinary sub-population, and a self-adaptive mechanism for dynamically adjusting algorithm parameters. Evaluations conducted on real-parameter CEC 2017 problems in various dimensional search spaces, compared against eleven state-of-the-art algorithms, consistently reveal the enhanced AEFA's superior performance in terms of solution accuracy, convergence rate, search capability, and stability. Overall, these strategies bolster AEFA's optimization capabilities, making it a potent tool for addressing intricate optimization challenges.

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PP1

Dynamic Bayesian History Matching

Computer models allow the study of complex systems and are widely applied in fields such as physics, engineering, and biology. History Matching (HM) is a statistical calibration method that considers all sources of uncertainty to provide a match between a model output and observed data. It explores the parameter space of a computer model, iteratively discarding regions that are unlikely to produce a reasonable output and generates samples from the non-implausible domain. However, HM only returns non-implausible regions and does not provide full Bayesian posterior distributions for the model parameters. Also, when new data is observed, HM cannot use previous information and must be run from the beginning. We propose incorporating sequential Monte Carlo methods with History Matching to provide full Bayesian posterior distributions for sequential calibration. We test our method in a cardio-respiratory model, by calibrating it to a continuous data stream from an intensive care unit from a hospital in London. We show that small perturbations to the non-implausible domain can be used sequentially.

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PP1

Experimental Validation of An Uncertainty Quantification Approach for Laser Powder Bed Fusion Additive Manufacturing

We present an efficient approach to quantify the uncertainties associated with the numerical simulations of the laser-based powder bed fusion of metals additive manufacturing process. Our study focuses on a thermomechanical model of an Inconel 625 cantilever beam, based on the AMBench2018-01 benchmark proposed by the National Institute of Standards and Technology (NIST). The proposed approach consists of an uncertainty quantification analysis of the numerical simulation parameters to reduce the uncertainties in the residual strains prediction of the cantilever beam. For this purpose, we use the data-informed probability density function of the powder convection coefficient and activation temperature obtained by a Bayesian inverse UQ analysis. To overcome the computational challenges of the uncertainty quantification analysis, we adopt multi-fidelity surrogate models using the multi-index stochastic collocation method. The proposed approach allows us to achieve a 40% reduction in the uncertainties associated with the prediction of residual strains, which tend to be in good agreement with the experimental data provided by NIST.

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PP1

Uncertainty Reduction in the Recognition of Dynamic Transients Within General Mixtures

Let us consider a general mixture, i.e. the sum of deterministic and stochastic signals, containing a set of known dynamic responses, e.g. transients from impulses applied to a mechanical system. In this talk we show how to recognize dynamic transients in general mixtures using a modified version of the DeepNMF algorithm. It relies mainly upon three features: discriminative initialization of the dictionary based on our prior knowledge of the physical system, enforcement of the time-correlation in the transients by projecting the forward-and-back-propagated factors into a block-Hankel space, and a modified loss-function that shifts the focus away from Wiener filtering in favor of a more accurate separation of the mixture contents. The recognition of dynamic transients is achieved by inspecting the H matrix, obtained by propagating the mixture spectrogram through the modified DeepNMF network, and computing an initial active index from ad-hoc averages on its entries. Since the latter are prone to stochastic noise, to reduce the uncertainty we introduce an appropriate latent space and posterior PDF for the recognition index within a Bayesian framework. The results show that by assuming multiplicative error models instead of the traditional additive ones, the Bayesian inference is able to provide more accurate and tighter confidence regions.

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PP1

Global Sensitivity Analysis of a Hybrid Pdeode Model for Cancer-on-Chip Experiments

Mathematical models are widely diffusing as instruments to study physiological/pathological phenomena as organogenesis, wound healing, tumor growth and invasion, or immune system response.However, the complexity of the interconnected processes at the basis of these phenomena may lead to mathematical models involving a large number of parameters, or parameters that are not directly measurable in vivo/vitro. In this context, the global sensitivity analysis offers methods to explore system behavior over a (even large) portion of the parameter space in order to: verify if the investigated region in the parameter space results in feasible scenarios; estimate how the parameters affect the variability of the outputs of the model. As a further result this approach can validate the model possibly suggesting further improvements or simplifications. In this work, this approach is applied to an extended version of the hybrid ODE-PDE model proposed in G. Bretti et al. (2021), built up to reproduce Cancer-on-chip experiments investigating the response of immune cells to chemical signals secreted by tumor cells treated with a chemotherapy drug. Several target outputs are considered in order to investigate either the spatial distribution and the dynamics of the immune cells. The sensitivity analysis is performed by first applying the Morris screening method dealing with 12 model parameters, and then eFast to compute the Sobol sensitivity indices of the 6 most important parameters.

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PP1

Deep Gaussian Processes for Surrogate Modeling with Categorical Data

Many applications of experimental design produce categorical response data. Popular classifiers such as neural network models can provide high predictive accuracy for examples with large input dimension. However, these models require large amounts of data and offer poor uncertainty quantification (UQ). This provides a challenge for situations where available training data is sparse. Gaussian processes (GP's) are stochastic models that can be modified to handle categorical responses and capture uncertainty with little training data. However, these models often struggle with non-stationary behavior in the form of rigid or asymmetric boundaries between classes. Deep Gaussian processes (DGP's) are functional compositions of GP's, and have excelled in regression settings for their ability to handle non-stationary behavior by warping the input space. We introduce a fully Bayesian implementation of the DGP model for multiclass classification. We show the DGP is preferable to the ordinary GP for modeling costly experimental designs with categorical responses.

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PP1

Sequential Construction of Block Additive Gaussian Processes under Inequality Constraints

Gaussian processes (GPs) are widely used in nonparametric Bayesian modeling since they provide both theoretical and computational benefits. Recent advances have improved predictive quality by introducing inequality constraints (e.g. monotonicity) to GPs, requiring the use of finite-dimensional GPs. However, those constrained models face challenges when dealing with functions involving more than 5 active variables. In response, constrained additive GPs, which are sums of 1-dimensional independent GPs, have emerged as a solution capable of handling hundreds of active variables. While they are computationally efficient and offer interpretability in real-world applications, they overlook variable interactions. Our presentation addresses these issues by introducing a framework for constrained block additive GPs. These GPs involve sums of multidimensional independent GPs with non-overlapping variable blocks, providing a solution for higher-dimensional functions while maintaining flexibility over their shapes. We also present a greedy algorithm, MaxMod which is used for model selection (choice of the blocks, finite-dimensional bases) and the construction of a function predictor.

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PP1

Adaptive Polynomial Chaos Expansion Methods for Vector-Valued Electric Machine Key Performance Indicators

Electric machine simulation is usually based on extremely time-consuming methods for precise approximations of typically vector-valued - key performance indicators (KPIs). In times of growing demand for efficient electric machine design and maintenance, surrogate models that replace expensive machine simulations while taking relevant uncertainties into account are of great benefit, both in the design process and during the life cycle of the electric machine. Therein, surrogate models can be used for fast prediction under uncertainty to accelerate the design process, while the life cycle of the machine can be enriched using digital twins, which consider uncertainties that influence the behavior of the machine in a non-deterministic way. In this work, we present different variants of adaptive polynomial chaos expansion (PCE) methods, which specifically target vector-valued quantities of interest, and discuss their performance in terms of accuracy and computation effort. The methods are tested on different electric machine models, where they are used to predict design and maintenance relevant KPIs. Possible extensions with active learning and prediction confidence measures will also be discussed.

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PP1

Comparison of Various Ordination Techniques in Understanding Spatially-Distributed River Microbiome Profiles

Microbiome datasets are often high dimensional, containing counts from a large number of different taxa. Dimensionality reduction techniques, also known as ordination techniques are utilized to visualize complex datasets in low dimensional space, while still maintaining a majority of the variability of the original dataset. This low dimensional representation is often easier to analyze, and is thus more amenable to identifying patterns and associations among samples. However, the implementation of ordination techniques is challenging for microbiome data due to their sparsity and compositionality. In this study, we considered a dataset containing bacterial profiles from different locations of the St. Lawrence River to compare the performance of three commonly used dimensionality reduction methods: principal coordinate analysis (PCOA), non-metric multidimensional scaling (NMDS), and t-distributed stochastic neighbor embedding (tSNE). A specific question of interest is the effect of sampling location versus river water bodies in bacterial composition. With all techniques, it appears that sampling location plays a more prominent role compared to water bodies. Among three techniques, NMDS clearly demonstrate the separation between the sample groups.Our findings confirm the utility of ordination methods to visualize and understand microbiome data and also suggest that different ordination techniques may be more appropriate for different questions of scientific interest.

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PP1

A Monte Carlo Scaling Study for Uncertainty Quantification Information Inequalities

In this poster presentation, we study properties of the Monte Carlo approximation for Uncertainty Quantification Information Inequalities (UQIIs). It is well-known that these inequalities are difficult to evaluate due to the instability in Monte Carlo approximation for exponential integrals. One approach that alleviates this issue is using a linearized form of the inequalities, which circumvents the need to estimate integrals of CGF type. However, it can be demonstrated that these linearized bounds fail when there is little data to ensure that the linearization is valid. This fact motivates this systematic study of the properties of the full UQIIs, and we find that with normal distributions as the underlying nominal and alternative models, we require a superexponential number of samples in the relative entropy ρ to expect that the optimization problems in the UQIIs have solutions.

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PP1

Bayesian Calibration of Innovative Air and Water Quality Sensors

More than 8 million people die each year as a result of air and water pollution, making it a major public health problem. In order to better monitor this pollution, this work aims to enable the deployment of innovative pollution measurement sensors. One difficulty in this deployment is the fact that the sensors we are working on are highly sensitive to pollutants but not very selective. This estimation is made challenging by the presence of many sources of uncertainty: the potential existence of unmeasured but influential pollutants, the measurement noises for the input and output data, and the fact that the relationship between sensors inputs and outputs is only partially learned. In order to integrate all these sources of uncertainty and make robust predictions, we propose to solve the problem using a Bayesian formalism. Two distinct phases are therefore needed for their use in uncontrolled environments. In the first step, the dependence of sensor responses on pollutant concentrations is estimated using labelled data provided by reference sensors. In the second step, this relationship is used to predict the pollutant concentration from the sensor outputs only. The performance of the proposed method is finally applied on simulated data and to air quality monitoring.

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PP1

A Comparison of the Determination of Active Variables in History Matching

History matching is a pre-calibration method used to rule out configurations of inputs which implausibly wont give output(s) near real world observations. When history matching on expensive numerical models, the quality of the emulation of the model is vital to ruling out space effectively. A key issue is the selection of variables to include as some may have little effect on the output (aka inactive variables). After one wave of history matching, the subspace not inconsistent with the data (aka NROYnot ruled out yetspace) is unlikely to have mutually independent inputs, so using classical sensitivity analysis methods to determine 'active variables are no longer appropriate. Alternatively, this determination has been done using automatic relevance determination, principal variables, stepwise regression, and LASSO. The common approach for determination of active variables is to use one of these methods on model runs sampled from NROY space. There can only be a limited number of samples to conduct these methods due to the computational expenditure of a model run. We investigate which of these methods provide the best solution with the small number of samples when compared to the 'best answer where these methods are applied to a much larger sample of points from NROY space. We do this comparison over many different NROY samples for multiple functions to see what the variability is in our answers and determine if there are any situations where a method outperforms another.

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PP1

Applying Optimal Experimental Design Techniques to High Energy Density Experiments

Many HED systems share the common problem of shocks interacting with interfaces which seeds the growth of hydrodynamic instabilities. These instabilities are a major degradation mechanism in inertial confinement fusion experiments, as they lead to asymmetry in target compression as well as mixing of "cold" material into the central hot spot. Understanding the growth and properties of these instabilities and how they transition to turbulence is important for many areas of research both in and outside of the HED context. HED experiments are expensive to preform, there are limited diagnostics available and experiments are typically multi-physics in nature. Additionally, new physics and uncertainties get introduced and the traditional theories break down. Such complexity means that modeling can become prohibitively expensive. Improving

the models from limited experimental data as well as and identifying informative experimental set ups is therefore of great importance. In this work we quantify and reduce uncertainty of model parameters inferred from Richtmyer-Meshkov (RM) and Rayleigh-Taylor (RT) experiments and apply optimal experimental design techniques to better understand how our initial conditions impact our results and identify the most informative experimental set ups for a given experimental goal. This work conducted under the auspices of the U.S. DOE by LANL under contract 89233218CNA000001

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PP1

Pce-Net: High Dimensional Surrogate Modeling for Learning Uncertainty

Learning data representations under uncertainty is an important task that emerges in numerous machine learning applications. However, uncertainty quantification (UQ) techniques are computationally intensive and become prohibitively expensive for high-dimensional data. In this paper, we present a novel surrogate model for representation learning and uncertainty quantification that aims to deal with data of moderate to high dimensions. The proposed model combines a neural network approach for dimensionality reduction of the (potentially high-dimensional) data, with a surrogate model method for learning the data distribution. We first employ a variational autoencoder (VAE) to learn a low-dimensional representation of the data distribution. We then propose to harness polynomial chaos expansion (PCE) formulation to map this distribution to the output target. The coefficients of PCE are learned from the distribution representation of the training data using a maximum mean discrepancy (MMD) approach. Our model enables us to (a) learn a representation of the data and a mapping between input and output distributions under uncertainty, (b) estimate the uncertainty in the high-dimensional data system, and (c) match high-order moments of the output distribution; without any prior statistical assumptions on the data. Numerical experimental results are presented to illustrate the performance of the proposed method.

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PP1

History Matching As a Calibration Method for Carbon Cycle Models

Simulators, complex physical models implemented in computer code, are a fundamental tool to assess ecosystem dynamics. Coupled with observational data, models can infer unobserved ecosystem properties. An example of this is the carbon cycle model DALEC Crop, which models the effect of Nitrogen fertilisation on wheat growth in a field over a crop growing season. Currently, DALEC Crops parameters are calibrated using a computationally costly Adaptive Proposal Markov Chain Monte Carlo algorithm. The current framework further does not allow for exploration of the effects of structural discrepancy and parametric uncertainty within the modelling framework. This in turn limits our understanding of the fields physical processes due to an underestimation of uncertainties when predicting yield or Leaf Nitrogen content. To facilitate quick model calibration and a thorough analysis of the uncertainties involved with DALEC Crop, this work presents history matching combined with emulation as an alternative to the current calibration framework. Using observations of Leaf Area Index when history matching allows us to find the set of input combinations for which the simulator gives acceptable matches to observed data. We demonstrate the suitability of the methodology building on previous work and data presented in [Revill et al., Agronomy, 2021]. An increase in possible outputs ranges highlights the need to explicitly account for uncertainties when assimilating observational data.

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PP1

Stability in Inverse Problems for the Generalized Schrdinger Equation

In inverse problems, the analysis of the stability is necessary before proceeding to the reconstruction because inverse problems are inherently ill-posed, lacking uniqueness and stability. Moreover, the presence of noise in the measurements or their incompleteness further complicates the reconstruction. The well-known ill-posedness nature of the problem can be overcome by introducing some a priori information that is physically meaningful. In this talk, we review recent results on the stability issue in both the coefficient identification problem and the inclusion determination problem. The direct problem is given by the generalised Schrdinger equation with Cauchy data as boundary data (infinitely many measurements). It includes, among others, the well-studied conductivity equation and the Schrdinger equation. Applications touch a variety of fields, including medical imaging, e.g. Electrical Impedance Tomography (EIT), a promising imaging technique based on the reconstruction of the conductivity and permittivity, geophysical prospection, e.g. Electrical Resistivity Tomography (ERT) based on the reconstruction of the resistivity, and non-destructive testing of materials.

We will show how the method of singular solution is successful in deriving optimal stability estimates and Lipschitz stability estimates from a small number of a priori information. This talk is partly based on a joint work with Eva Sincich.

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PP1

Hierarchical Sequential Monte Carlo Algorithms in Personalized Medicine

In Data Assimilation, Hierarchical Sequential Monte Carlo algorithms are used for simultaneously estimating state and parameter. The application of such methods is wide and ranges from robotics to financing. In personalized medicine, similar problems arise for models related to treatment. Batch methods are often not applicable due to data protection laws. In many countries, data protection laws prohibit the storage of data in a center location, which hampers batch updates of state and parameter. Sequential methods can provide a solution. There are already attempts to use similar methods to Hierarchical Sequential Monte Carlo in personalized medicine. For these algorithms, there is limited evidence available that they even work in the applied cases. Based on Bayesian Data Assimilation and Machine Learning, we explore new algorithmic ideas to tackle the problem outlined above.

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PP1

Surrogate Modelling for Non-Linear Partial Differential Equations

Partial differential equations (PDEs) are used to model many physical problems. Most of the time, analytical solutions u of PDEs are unknown and they are solved with numerical methods, let denote u_{num} this solution. These methods can be expensive in computation time and in some cases inaccurate (approximate physics, choice of numerical parameters, ...). To reduce computational time, an alternative is to replace this numerical solution u_{num} by an approximation, called surrogate model, built from pointwise evaluations of u_{num}. In order to correct the error made by introducing u_{num} instead of u, we propose an adaptive method which integrates the PDE in the construction of the model. The objective of this work is to obtain an approximation of u more accurate and faster than u_{num}. This method is applied for the Burger's equation to two approximation tools: Gaussian process regression and tree-based tensor formats.

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PP1

Edge-Preserving Tomographic Reconstruction with Uncertain View Angles

In computed tomography, data consist of measurements of the attenuation of X-rays passing through an object. The goal is to reconstruct an image of the linear attenuation coefficient of the object's interior. For each position of the X-ray source, characterized by its angle with respect to a fixed coordinate system, one measures a set of data referred to as a view. A common assumption is that these view angles are known but in some applications, they are known with imprecision. We present a Bayesian inference approach to solving the joint inverse problem for the image and the view angles, while also providing uncertainty estimates. For the image, we impose a Laplace difference prior enabling the representation of sharp edges in the image; this prior has connections to total variation regularization. For the view angles, we use a von Mises prior which is a 2π-periodic continuous probability distribution. Numerical results show that our algorithm can jointly identify the image and the view angles, while also providing uncertainty estimates of both. We illustrate our method with simulations of a 2D X-ray computed tomography problems using fan beam configurations.

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PP1

Deep Gaussian Process Emulation and a Hierarchical Calibration Framework for a Complex Farm Model Incorporating Uncertainties

Computer models used in agricultural systems often have

numerous site-specific model parameters, large forcing data sets and can be expensive to run. For example, our simulator, WOFOST, simulates field-parcel crop yields, given species specific parameters (shared across all land parcels), as well as soil moisture and nutrient content in the field, daily weather data (historical or projected into the future), soil type and farm-specific management (timing and level of fertiliser application). We present the performance of deep Gaussian process emulators with active subspaces for WOFOST and compare them to standard emulation approaches. We then develop a hierarchical calibration framework for sharing our limited yield data on $3,500$ farms across the $\sim$ 250000 field parcels in the UK, for quantifying uncertainty in the field specific parameters. We demonstrate the potential of this technology for creating self-updating digital twins for large collections of farms in the UK.

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PP1

Uncertainty Quantification for a Posterior with Besov Prior

In Bayesian inverse problems, the prior distribution incorporates a priori information about the unknown quantity into the inverse problem. The choice of prior distribution can be crucial for the estimation of the unknown quantity. Besov priors is a family of wavelet-based priors that can promote both smooth and non-smooth function regularity. In this talk, we use sampling methods to study uncertainty quantification for a posterior with Besov prior. We adapt the posterior with Besov prior to be applicable for the Randomize-Then-Optimize sampler, which we use to explore how specific choices of Besov prior affect the uncertainty quantification of the posterior in illustrative inverse problems.

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PP1

Uncertainty Quantification on Time Series Forecasting

Time series forecasting is one of the most sophisticated statistical methodologies that has been utilized as the state of art of decision-making strategies in every underlying stochastic phenomenon. However, uncertainty is an intrinsic ingredient of time series forecasting process which can be greatly affected towards the end results of the forecast. In case of data uncertainty each of the available time series models behave differently for specific characteristics of the time series data, that is Trend, Seasonality, Sparsity, etc. On the other hand, once we developed a time series model for a given set of data and how its performance for unseen data, is called uncertainty with respect to the model. Identifying the robust model with respect to data uncertainty or model uncertainty will improve the results significantly and forecasters can make strategic decisions based on the results of a highly reliable model. Thus, in this study we will answer the following two questions by utilizing traditional and modern forecasting methodologies such as ARIMA, Hawkes Process, LSTM and Transformers and time series data with specific characteristic of Trend, Seasonality, Sparsity, Cyclic behavior, etc. and will utilize the sophisticated statistical methods to validate the high quality of the proposed uncertainty quantification. These questions are, I) How to minimize Data Uncertainty in time series forecasting? II) How to minimize Model Uncertainty in time series forecasting?

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PP1

Multilevel Monte Carlo Methods for Chaotic Systems

We consider the computational efficiency of the Multilevel Monte Carlo (MLMC) algorithm applied to chaotic systems of the form $x'(t) = f(x(t))$, $t \in [0, T]$. Here, $f : \mathbb{R}^m \to \mathbb{R}^m$ is a Lipschitz function satisfying the dissipativity condition, but not the following contractivity condition:

$$\langle x - y, f(x) - f(y) \rangle \leq -\lambda \|x - y\|^2, \quad \forall x, y \in \mathbb{R}^m. \quad (3)$$

A direct application of MLMC to such systems is challenging due to the exponential increase of the variance of the level estimators with respect to the final time, T, and hence of the corresponding computational complexity. To alleviate this issue, Fang and Giles [1] proposed the change of measure technique for the stochastic variant of the deterministic dynamical system, which recovers the contractivity of the path. Building on their work, our aim is to compute quantities of interest of the deterministic system with and without random coefficients, using its stochastic variant as a control variate. We apply our method to Lorenz63, a three-dimensional system modelling convection rolls in the atmosphere. [1] W. Fang, M. Giles, Multilevel Monte Carlo method for ergodic SDEs without contractivity, *J. Math. Anal. Appl.* 476 (2019) 149176

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PP1

Learning Active Subspaces for Effective and Scalable Uncertainty Quantification in Deep Neural Networks

Bayesian inference for neural networks, or Bayesian deep learning, has the potential to provide well-calibrated predictions with quantified uncertainty and robustness. However, the main hurdle for Bayesian deep learning is its computational complexity due to the high dimensionality of the parameter space. In this work, we propose a novel scheme that addresses this limitation by constructing a low-dimensional subspace of the neural network parameters–referred to as an *active subspace*–by identifying the parameter directions that have the most significant influence on the output of the neural network. We demonstrate that the significantly reduced active subspace enables effective and scalable Bayesian inference via either Monte Carlo (MC) sampling methods, otherwise computationally intractable, or variational inference. Empirically, our approach provides reliable predictions with robust uncertainty estimates for various regression tasks.

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PP1

Towards Predictive Uncertainty Quantification in Space Weather Simulations Through Surrogate Models for Dynamical Systems

Uncertainty Quantification (UQ) is critical in applications involving computationally expensive simulations of field quantities of interest. One example domain is that of Space Weather, where predictive models are built from first principles to simulate phenomena such as CMEs (coronal mass ejections) and forecast their arrival time as well as geomagnetic impact. The processed QoIs from the simulations are then validated against remote and in-situ observations. The high cost of simulating Sun-to-Earth propagation of CMEs for a new event restricts access to only a limited number of simulations based on varying flux rope parameters that describe the strength and shape of the CME. In this setting, surrogate models or emulators for approximating the true dynamics are valuable tools to provide improved extrapolation of the training data at arbitrary timesteps. These can also accelerate forward UQ to propagate uncertainty from the free parameters to the QoIs and the subsequent inverse UQ step for constraining the parameters. Here, we compare the performance of 3 emulators Proper Orthogonal Decomposition (POD), Operator Inference (OpInf) and Neural Ordinary Differential Equations (NODEs). These are constructed using data from synthetic white light images and derived 1D CME leading edges. The final surrogate model can be used for generating the evolution of the leading edge based on unseen initial conditions and also supply predictive uncertainties on the test simulations.

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PP1

Real-Time Optimisation of Speed Control to Limit Train Energy Consumption Using Manifold Learning

Reducing ecological footprint has become a priority for most industries including the railway industry which is one of the most energy-consuming industry. In that prospect, the optimisation of the drivers control to reduce the consumed energy while respecting multiple constraints (punctuality, security, etc.) is a particularly important challenge. Several proposals for optimising these control functions can therefore be found in the literature, mainly based on offline methods to guide the driver toward optimality. Continuing these works, this presentation focuses on an online methodology to make use of the knowledge brought by on-board sensors. Focusing on a particular type of train, and for a particular track, this work breaks down into four phases: the implementation of a simplified parametric model of the train, the estimation of the parameters of this model by Bayesian inference from dedicated online measurements, the offline approximation of the manifold characterising the set of optimal controls associated with the set of likely values of the model parameters, and then an online method for updating the true controls of the true train as it runs, by combining the information provided by this manifold with the position and speed measurements recorded in real time. Finally, the efficiency and the robustness of the method are numerically validated using nominal and non-nominal contexts.

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PP1

Inverse Stochastic Microstructure Design

Materials science is full of inverse problems. For example, designing manufacturable materials given a set of target properties requires inverting the complex linkages from processing parameters to microstructure to property. This inversion is complicated by the high-dimensional, disordered nature of microstructures, as well as ill-conditioning in the inversion process and a scarcity of well-sampled datasets. In this work, we propose a Bayesian framework for materials inverse problems. We leverage machine learning models to estimate prior and likelihood distributions, culminating in a stochastic Variational Inference procedure for the inverse Structure ¡- Property linkage. In particular, we demonstrate how one can embed domain knowledge (via statistical continuum mechanics) into a low-dimensional, property-independent microstructure prior. We apply our model to the problem of designing woven ceramic-matrix composites given a target set of anisotropic thermal conductivities. Additionally, we test the model's calibration across a number of increasingly-difficult test cases and its stability outside the training distribution. Finally, we explore the utility of our framework for problems such as uncertainty propagation and amortized learning.

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PP1

Sampling Low-Fidelity Outputs for Estimation of High-Fidelity Density and Its Tails

In a multifidelity setting, data are available under the same conditions from two (or more) sources, e.g. computer codes, one being lower-fidelity but computationally cheaper, and the other higher-fidelity and more expensive. This work studies for which low-fidelity outputs, one should obtain high-fidelity outputs, if the goal is to estimate the probability density function of the latter, especially when it comes to the distribution tails and extremes. It is suggested to approach this problem from the perspective of the importance sampling of low-fidelity outputs according to some proposal distribution, combined with special considerations for the distribution tails based on extreme value theory. The notion of an optimal proposal distribution is introduced and investigated, in both theory and simulations. The approach is motivated and illustrated with an application to estimate the probability density function of record extremes of ship motions, obtained through two computer codes of different fidelities and speeds.

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PP1

Exploring Biomineralization Properties Through Surrogate Models and Bayesian Model Comparison

Bayesian model comparison helps choose models that are of appropriate complexity given experimental data. We are focusing on biomineralization via enzymatically induced calcium carbonate precipitation (EICP). To use this process to its full potential we need detailed descriptions of where the calcium carbonate will precipitate. This is hindered by the formation of flow paths, the causes for which are not yet fully understood. In addition, mobile precursor phases to stable calcium carbonate polymorphs influence the precipitation distribution in ways that are difficult to characterize on the REV scale. We extend an REV scale reactive transport model for EICP to account for the transformation from the instable precursor amorphous calcium carbonate (ACC) to calcite and the interplay of ACC with its surroundings. As the models often come with a higher computational cost than feasible for Monte-Carlo evaluations, surrogate models are used to replace them. In this scope we replace the full physical model by an arbitrary Polynomial Chaos Expansion and train it on samples chosen by Bayesian Active Learning. By applying Bayesian model comparison to a discrete set of variations of this model we draw conclusions about the attachment and detachment processes of ACC. Comparing our models to experimental data allows us to identify key features of ACC behaviour and the formation of flow paths during biomineralization.

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PP1

Triangular Transport Maps on Bounded Domains

Measure transport underlies many powerful and flexible methods for representing complex probability distributions. Triangular transport maps are a particularly useful choice in this context, as they are computationally tractable and well-suited to conditional simulation and conditional density estimation, with applications in Bayesian inference. For distributions supported on unbounded domains, Baptista et al. (2022) propose a general framework for representing and learning monotone triangular maps (approximations of the Knothe–Rosenblatt (KR) rearrangement) from samples of the target distribution. Yet many settings involve hard constraints on the range of the variables of interest, such that transport methods formulated on unbounded domains work poorly, as they create samples outside of the feasible region. In this work, we introduce a computational framework to learn KR rearrangements for distributions supported on *bounded* domains. To do so, we rely on a rational parameterization of the transport map (see Zech & Marzouk 2022, Wang & Marzouk 2022) that automatically satisfies the monotonicity and range constraints of the bounded setting. Under appropriate conditions on the reference distribution, we show that maximum likelihood estimation of the transport yields a set of convex optimization problems that can be solved independently. We demonstrate the performance of this new framework on examples of density estimation from few samples.

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PP1

A Unified Workflow for Bayesian Model Selection.

The existence of a myriad of competing computational models in a wide range of scientific and engineering applications poses a formidable challenge when selecting the most plausible model for a given set of observations. Quantifying the uncertainty associated with this model selection process is essential for assessing the reliability of the predictions of these computational models. Here, we introduce a unified Bayesian model selection workflow. It starts with model calibration, where we generate posterior samples. These are then used to calculate the marginal likelihood, the basis for our model selection. This process faces two computational bottlenecks: significant computational costs involved in numerous model evaluations during calibration and high-dimensional, intractable integrals in the computation of Marginal Likelihood. To address the former, we integrated Gaussian process emulators into the workflow using PSimPy, our in-house Python package, for predictive and probabilistic simulations. For the latter bottleneck, we employed techniques based on Importance Sampling. We demonstrate this approach using elementary landslide runout models with varying fidelity levels, investigating the effects of data representation (point data vs. time series data) and data characteristics such as velocity and distance. Furthermore, we explored the calibration of the discrepancy parameter for robust handling of model inadequacy and measurement noise uncertainties.

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PP1

Invariant-Preserving Ensemble Filters for Conservation Laws

Conservation laws are an important class of evolution equations to model geophysical and atmospheric phenomena. Unfortunately, a dynamical model alone is often insufficient to track the evolution of these systems. Indeed, the dynamical model suffers from model errors and uncertainties. One common remedy is to rely on data assimilation, where the state estimate is updated with observations of the true system. Ensemble filters sequentially assimilate observations by updating a set of samples over time. They operate in two steps: a forecast step that propagates each sample through the dynamical model, and an analysis step that updates the samples with incoming observations. For accurate and robust predictions of conservations laws, discrete solutions must preserve their critical invariants. While modern numerical solvers satisfy these invariants, existing invariant-preserving analysis steps are costly and often not compatible with classical regularization techniques of ensemble filters, e.g., inflation and localization. In this work, we interpret these invariant conditions as implicit parameterizations of particular manifolds. Using explicit coordinate systems for these manifolds, we show how to transform the analysis step of a generic ensemble filter

to automatically satisfy these constraints. We assess the benefits of this methodology on several conservation laws.

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PP1

Multiple Inputs Fourier Neural Operator for 3D Elastic Wave Propagation

Physics-based simulations are necessary to solve numerous Partial Differential Equations (PDEs) but they are generally unsuitable for uncertainty quantification due to their high computational costs. This is especially true when dealing with high-dimensional variables. This work focuses on the propagation of seismic waves in the ground to quantify the influence of geological uncertainties and seismic source on surface ground motion. Geologies are represented by three-dimensional (3D) domains discretized in tens of thousands of voxels to model small-scale heterogeneities perturbing the propagation of waves. We trained Fourier Neural Operators (FNOs) on a database of 30,000 pairs of geologies with their associated ground motion. Additionally, we explored the advantages of dimensionality reduction to include source effects inside our surrogate model. We show that Fourier Neural Operators (FNO) are accurate surrogate models to predict 3D surface ground motion and we compare several FNO variants to improve the high-frequency predictions. Thanks to the low inference time of neural networks, FNO predictions are used to derive confidence intervals of ground motion intensity measures. They yield security margins compared to the usual methods in seismic hazard analyses, making them worth consideration for uncertainty quantification in real applications.

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PP1

Understanding the Effects of Model Uncertainty and Data Variability for Predictive Modeling in Diabetes

Predictive modeling plays an essential role in diagnosing diabetes and predicting the effects of medical treatments by allowing clinicians to make inferences about a patients metabolic health from clinical data. For example, the oral glucose tolerance test (OGTT) helps determine how a patients pancreas responds to a perturbation in blood glucose, the signal that drives pancreatic insulin release. Glucose-driven pancreatic insulin secretion has been represented with a set of related mathematical models that predict pancreatic responsiveness and sensitivity to glucose from OGTT data. However, these predictions often come without a quantitative assessment of the associated uncertainty. In this poster, we leverage multimodel inference, also called model averaging or model fusion, and global sensitivity analysis to probe how uncertainty in the model formulation and variability in the data affect model-based predictions of pancreatic function. Here, we show how tools from UQ can bring valuable insights to predictive modeling in the clinic and inform clinical test designs to minimize predictive uncertainties.

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PP1

The Use of Machine Learning Analysis for Fraud Prediction in Car Insurance Claims

The objective of this research is to compare the performance of four models, including three machine learning analysis methods: Nave Bayes, XGBoost, and Random Forest, and a statistical method: Logistic Regression. These models were created to detect fraudulent claims for car insurance and predict whether a person who claims insurance is likely to commit fraud. The data used for this research consists of car insurance claim data from a car insurance company in the United States between the years 1994 and 1996, with a total of 15,420 individuals. The problem of imbalanced data between variables was addressed using the Combining Over-Sampling and Under-Sampling Techniques method. The XGBoost method was found to have the most accurate and efficient prediction with an accuracy of 0.9608, precision of 1.0000, recall of 0.9267, F1-score of 0.9620, and AUC of 0.992.

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PP1

Global Sensitivity Analysis of a Pollutant Dispersion Uncertainty Quantification Problem

Air pollution is a pressing issue challenging modern society

from both public health and environmental perspectives. The latest World Health Organisation (WHO) data shows that more than 90% of the world population "breathes air that exceeds WHO guideline limits" and each year 4.2 million deaths can be linked to ambient air pollution. Computational modelling enables the study of model parameters and physical processes in pollutant dispersion models in order to gain some insight into the factors that strongly influence atmospheric pollution concentration. In this talk we consider a parametric advection-diffusion pollution dispersion model to investigate how the pollutant concentration varies with respect to uncertainty or variability in the model parameters. A global sensitivity analysis (GSA) is conducted to assess how the variability in the pollutant concentration can be attributed to the variability in the model parameters. We use a variance-based GSA technique based on the estimation of first order and total Sobol indices across the spatial domain using Monte-Carlo sampling. To improve the computational efficiency of this approach we present improvements which can be obtained using a control-variate method using a combination of high and low fidelity models for variance reduction. Result will be presented using low fidelity models based on coarse finite element meshes and surrogate models based on Gaussian processes.

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PP1

A Case Study on Municipal Solid Waste Management Problem under Uncertain Environment

This paper investigates a case study of municipal solid waste management to minimize the cost of waste transportation, cost of waste treatment and maximize the revenue generated from various treatment facilities with real life parameters represented as uncertain numbers. The model includes the knowledge and agreement as well as difference in judgements of all the experts involved. To deal with the conflicting nature of different objectives, a nonlinear membership function for each objective is introduced and an approach is developed that gives the optimistic and pessimistic view of the decision-maker in optimizing the proposed model. Finally, to demonstrate the practicality of the proposed approach, a case study is solved, and the obtained results are analyzed and discussed.

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PP1

Oblique Projection for Fast Implicit Integration on Low-Rank Matrix Manifolds

Discretization of random time-dependent PDEs results in massive matrix differential equations (MDEs) whose numerical solution is prohibitively expensive. Low-rank approximation via time-dependent bases (TDB) has proven highly effective for model reduction of these MDEs. However, most TDB techniques are limited to explicit integration. This work presents an efficient implicit integration approach for large-scale MDEs based on TDB within a matrix CUR framework. The key innovations are: 1) Sparse sampling to achieve linear computational scaling with system size, 2) Simple non-intrusive deployment by treating operators as black boxes, and 3) Adaptive rank adjustment controlling the approximation error. TDB-CUR interpolates important column and row spaces over time, avoiding costly repeated decompositions. Numerical experiments on analytical MDEs and PDEs, including stochastic Burgers' and Gray-Scott equations, demonstrate substantial speedups over full integration. This enables extending TDB model reduction to stiff systems requiring implicit integration in an efficient and scalable manner.

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PP1

Probabilistic and Generative Machine Learning to Estimate Predictability and Quantify Uncertainty

While predictive modeling of complex, multiscale nonlinear dynamical systems, irrespective of whether they are natural or engineered, is predicated on the various sources of predictability, essential to rendering such modeling reliable and robust is a comprehensive consideration of the various sources of uncertainty. While predictability typically arises from deterministic dynamics, dynamical symmetries (with their associated invariants), and various linear, nonlinear and emergent oscillations/patterns (e.g., in the climate system, the annual seasonal cycle, Rossby waves, the North Atlantic Oscillation, the El Nino Southern Oscillation, the Atlantic Meridional Overturning Circulation, etc.), sources of uncertainty include model uncertainty—structural and parametric—that may arise in part due to computational resource limitations, and initial and boundary condition uncertainty. This talk will consider the use of probabilistic and generative machine learning techniques in better estimating predictability characteristics and better quantifying uncertainty in predictions of complex systems. Results using Generative Adversarial Networks, Variational Autoencoders, Reservoir Computing, and attention-based transformers will be presented and discussed.

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PP1

Categorical Output Model Emulation with Deep Gaussian Processes.

Digital twins (DTs) combine computer models aimed at replicating the behaviour of a physical system with often real-time data streams to assist decision makers. To enable real-time performance, expensive components can be 'emulated' by statistical machine learning models known as emulators or surrogate models. Surrogate models often rely on neural networks or Gaussian Processes (GPs), the former being better adapted to relatively inexpensive models where large training sets are available. For very expensive computations, GP surrogates are usually favoured. In this talk, we present a novel GP formulation for capturing spatial fields of categorical variables. This work is inspired by an application to policy support for tree planting incentivisation schemes in the UK where the model outputs are maps composed of cells whose values are a type of tree planted. Our method performs a latent singular value decomposition that enables a handful of GP coefficients to be emulated in order to reconstruct categorical predictions with uncertainty. We show how sequential design can be used to train the coefficients to deliver a desired accuracy as efficiently as possible. We apply our method to the tree planting incentivisation problem and argue that deep Gaussian process emulators for the coefficients are, in our practical experience, more accurate than the typically used stationary GPs.

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PP1

Long-Term Dynamics of the Kidney Disease Epidemic Among Hiv-Infected Individuals

One of many risks facing HIV_+ individuals is the development of kidney dysfunction and end stage kidney disease (ESKD). A differential equation-based mathematical model was developed to assess the impact of antiretroviral therapy on the progression to kidney disease and on reducing mortality due to kidney failure. Analytical and numerical predictions of long-term HIV_+ ESKD prevalence show that therapy can lead to either extremely low levels of disease prevalence or increased prevalence, depending on drug efficacy levels and mechanisms of action. Maintenance of HIV_+ ESKD prevalence below one individual is possible with sufficient efficacy (e.g., 99%) against the progression from AIDS to HIV_+ ESKD and against entry to the AIDS population, when the reduction in mortality in the AIDS and HIV_+ ESKD populations is modest (e.g., 10%). However, the concomitant decrease in mortality in the AIDS and HIV_+ ESKD populations due to therapy is predicted to sustain greater disease prevalence.

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PP1

Maximal Parameter Estimates for Neural Networks and Uncertainties in Approximation

We take a structural description of neural networks first proposed by Peterson and Voightlander, 2019 and further built upon by Grohs et. al, 2020, and further extend this neural network calculus. Along the way we rebuild several bits of well-known machinery in the language of neural networks and show that yes, indeed, parameter estimates are bounded polynomially on the precision of our estimates. We give: 1. Neural network architectures representing Taylor polynomials and e^x. 2. Neural network architectures that are able to simulate a highly modified Monte Carlo sampling from Brownian motions along the function support 3. Neural network estimates for trapezoidal rule 4. And finally for the first time, that neural networks without too many (defined as being polynomial on the precision) parameters may be able to approximate a modified diffusion equation. This adds to the literature in that it builds upon a much needed need to formally axiomatize neural networks, both in terms of the number of parameters and exactly how expressive it can be. Minimal parameter estimates mean neural networks will be more accessible in smaller computing devices, meaning greater access for more people to this amazing technology and it means that more efficient neural networks can be built which reduce environmental impact as we march forward into a more artificial intelligence focused age.

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PP1

Probablistic Validation of a Cable Photocurrent Model

Verification and validation are two distinct fields that are vital to the assessment of performance and reliability of numerical models. We distinguish verification and validation by referencing the commmon sentiments; verification is demonstrating one has "solved equations properly" while validation showcases that the model "solves the right equations." In this poster, we perform model validation, by applying a variety of validation metrics to a cable photocurrent model, with comparison to experiment from the Pithon acelerator. In particular, we compare these various validation metrics to each other, among other traditional metrics. Importantly, we demonstrate that the inclusion of uncertainty (both of an epistemic and aleatoric nature) is cricitcal in the assessment of a model's capabilities, particularly from a validation viewpoint. To that end, we also discuss how different approaches to validation handle these different types of uncertainty, and present both de-

terministic and probabilistic validation metrics. Finally, we demonstrate both the importance of uncertainty and of detailed experimental accountings when performing robust model validation. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

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PP1

Multi-Fidelity Sensitivity Analysis for Plasma Micro-Instability Using Gaussian Process

The high computational cost of the models is one of the significant hurdles for performing the forward uncertainty quantification (UQ) analysis. To overcome this problem, we use multi-fidelity modeling within the forward UQ setup. We combine the information from different hierarchies of fidelities to obtain the statistical moments of the highest fidelity model by consuming low computational resources. We use the Gaussian Process (GP) to build a multi-fidelity surrogate. We then use this surrogate to estimate the Sobol-sensitivity index. We use the multi-fidelity rank-based estimator to ensure unbiasedness of the statistical moments with respect to the high-fidelity model. We apply the proposed method to Plasma micro-instability problems. The analysis provides crucial information for the Plasma-physics community regarding plasma behavior under specified conditions.

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PP1

Uncertainty Quantification and Propagation in Surrogate-Based Bayesian Inference

Surrogate models are statistical or conceptual approximations for highly complex simulations. In this context, it is crucial to propagate the uncertainty due to limited simulations and due to the approximation error of the surrogate model to predictions and subsequent decision-relevant quantities. However, quantifying the uncertainty of surrogates is usually limited to the use of special analytic cases or is otherwise computationally very expensive. We propose a framework allowing a scalable, fully Bayesian approach to surrogate modeling with uncertainty propagation and its evaluation. We also present three methods for Bayesian inference with surrogate models given measurement data a task where the propagation of surrogate uncertainty is especially relevant, because failing to account for it may lead to biased and/or overconfident estimates of the unknown simulation parameters. Finally, we validate our Bayesian inference on easy-to-visualize case studies with varying complexity ranging from linear models to complex nonlinear models. Uncertainty propagation in surrogate models enables more reliable and safe approximation of expensive simulations and will therefore be useful in various fields of applications, such as systems biology, molecular dynamics, or fluid dynamics.

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PP1

Data to Improve the Representation of Wind in Hurricane Storm Surge Modeling

Storm surge models are vital tools for understanding the risk that surges pose to coastal communities as sea levels rise and hurricanes intensify. These models are integral to both real-time forecasting of surge behaviors during a weather event and long-term planning of adequate surge preparation. The accuracy of surge prediction models such as ADCIRC is substantially dependent on wind field representations, but accessing the most robust models is not always computationally feasible. High-quality wind models are generally not capable of real-time forecasting, so fine details are often sacrificed in lieu of a few key parameters. This leads to the usage of parametric models that contain a small number of parameters such as intensity, size, and track location to represent wind, which is more tractable but not as accurate to the true wind behavior. In this work, we aim to improve the modeling system of wind and surge as a whole using data. We implement methods to minimize uncertainties regardless of wind model accuracy and address whether data assimilation can viably improve wind field representation for forecasting and hind-casting. We assess the loss of accuracy from parametric wind models, then attempt to mitigate the loss with assimilation of high-fidelity wind data within a parametric framework. This work has the potential to help with poor wind field representation for real-time and hindcasting and produce more accurate predictions of hurricane storm surges.

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PP1

A Novel Constrained Design of Experiments Technique Incorporating Experimental Knowledge for Computationally Guided Materials Experimentation

The time and money required to discover a new functional material, or optimize a known one by a factor of ten, is estimated to be ten million dollars and ten years. Materials research faces a myriad of efficiency-related challenges, including resource management, data collection, and exploration of new material compositions. Additionally, the quest for optimal material compositions introduces further complexities, such as incorporating problem-specific constraints. In this talk, we introduce a novel constrained design of experiments strategy designed to construct an optimal dataset for the exploration of the design space that integrates existing experimental knowledge while exploring a multidimensional constrained input space and preserving uniformity. This novel technique provides a feasible amount of recommended experiments to be executed by the experimentalist for the exploration of the design space. The value of these novel algorithmic developments will be demonstrated by their employment for strategic planning and execution of experiments for materials design and show how this can be incorporated in robotically automated and accelerated experiments. This work gives a glimpse of the transformative potential of optimal autonomous experimentation including uncertainty quantification and new algorithmic developments in advancing materials research.

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PP1

An R Implementation of Adaptive Marginal Likelihood Sampling for Bayesian Model Selection

In Bin Liu's 2014 paper *Adaptive Annealed Importance Sampling for Multimodal Posterior Exploration and Model Selection with Application to Extrasolar Planet Detection*, he introduces an algorithm that can adaptively provide mixture summaries of multimodal posterior distributions. For Bayesian model comparison, one needs to evaluate marginal likelihoods which is notoriously dificult because models are often highly nonlinear and multimodal. Importance sampling is powerful technique for estimating integrals, but finding importance functions that mimic the integrand is challenging in high-dimensional problems. In order to capture the multimodal structure of the models, this algorithm employs mixture distributions, which are adaptively added, deleted, and merged with to approximate the target distributions. Further, the parameters of these mixture components are updated via expectation-maximization. Code accompanying this paper was written in MATLAB. We will present a new R implementation, and demonstrate the algorithm on both challenging target functions and Bayesian model selection examples.

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PP1

Estimating the Effective Sample Size for An Inverse Problem in Subsurface Flows

The Bayesian approach to solving an inverse problem in subsurface flows requires Markov Chain Monte Carlo (MCMC) methods. The objective of this project is to use the Effective Sample Size (ESS) and Integrated Autocorrelation Time (IACT) to compare two different such MCMC methods and analyze their output. The main difficulty we have encountered is that there are many distinct approaches to estimate the ESS and IACT, and it is not clear which method would be more appropriate for our problem. We therefore consider a few estimators that are part of popular software packages. Those are the Bulk-ESS, Batch Means, AR(p) fitting, Tukey Window and Bartlett Window. To gain some insight, we first use simulations of 100 independent AR(1) chains with specific IACTs to visualize the empirical distribution of each estimator mentioned above. This is done for an IACT of 5000 and then 50000. From here, we notice that the estimators for the ESS may not be consistent in the statistical sense. Then, we consider a linear elliptic inverse problem that recovers a permeability field given noisy measurements of the pressure. The two MCMC methods tested are a two-stage MCMC method and a multiscale MCMC method. We notice that the estimators for the IACT might not even agree in the order of magnitude. We then conclude our project by giving reasons why that may be so, and recommend reporting the Monte Carlo Standard Error or IACT instead of the ESS in papers.

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PP1

Mitigating Overconfidence in Bayesian Field Inversion Using Hyperparameters Space Exploration

In this work, we are interested in estimating a scalar field from noisy indirect observations. In order to obtain a full posterior distribution of the quantity of interest, the inverse problem is formulated in a Bayesian framework along with Markov chain Monte Carlo sampling. Inferring a field is expensive with regard to its infinite dimension and to the forward model computational cost. Our approach relies on a parametrization based on the Karhunen-Love decomposition. Although attractive since it provides a representation with a finite number of terms, the KL decomposition depends on the hyperparameters of its autocovariance function that are difficult to choose a priori due to lack

of knowledge. Instead of selecting deterministic values, we propose to deal with hyperparameters prior distributions in order to test various field shapes during the sampling. For that purpose, we present a novel approach based on a change of measure of the decomposition coordinates that allows a smooth exploration of the hyperparameter space. Our sampling procedure is accelerated by means of polynomial chaos expansions to replace the data computed from the forward model. Our method is applied to a transient diffusion problem, the results are similar to those obtained with previous approaches. A seismic traveltime tomography case shows that exploring the hyperparameters space improves the uncertainty estimation compared to the approach with fixed hyperparameters.

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PP1

Sequential Maximal Updated Density Parameter Estimation for Dynamical Systems with Parameter Drift

We introduce novel methods to produce sequential parameter estimates and quantify epistemic uncertainty in dynamical systems, building on prior work that derives a parameter estimate, akin to a Bayesian (MAP) point, using data-constructed maps on residuals between observed and model values. The update to prior beliefs uses a Data-Consistent (DC) model, leveraging a stochastic forward problem (SFP) solution. This updates the initial density based on model output data, selectively regularizing in the parameter directions not informed by the data. We enhance previous DC parameter estimation methods by considering sequential techniques, using past updates to inform subsequent ones, and introduce the relevant updating algorithms. We demonstrate how established metrics for evaluating DC updates and information gain can be used to assess sequential parameter estimations, especially in detecting parameter drift. We apply the presented algorithms to three dynamical system parameter estimation problems: wind drag in a high-fidelity storm surge model, thermal diffusivity in a heat conductivity problem, and changing infection and incubation rates in an epidemiological model. Results demonstrate DC methods' potential for real-time uncertainty quantification as packets of noisy observational data is obtained from sensor networks. The algorithms introduced here provide a foundation for expanding Data-Consistent parameter estimation into more conventional data-assimilation methods.

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PP1

Alpha-Stable Priors in Bayesian Inversion

Lvy alpha-stable distributions are a class of probability distributions used to model various phenomena in science and engineering because they are closed under convolution and typically heavy-tailed. However, the probability density functions of alpha-stable distributions cannot be expressed through elementary functions besides a few expectations including the Gaussian and Cauchy distributions. Our objective is to incorporate numerically feasible approximations of Lvy alpha-stable processes in Bayesian inversion. To that end, we introduce a hybrid method to approximate the log probability density functions of univariate and symmetrically contoured alpha-stable distributions. The method incorporates bicubic splines on a precomputed grid of alpha-stable densities, and it also employs asymptotic series expansions of the alpha-stable probability density functions. In contrast to the existing approximation approaches, our method is fast to evaluate and usable on a continuous range of the stability indices with an arbitrary argument of the probability density function. We demonstrate the novel features of the alpha-stable processes and the applicability of our approximation method as part of a Bayesian inverse problem.

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PP1

Rigorous Analysis of the Ensemble Transform Kalman Filter for Chaotic Dynamical Models

The process of data assimilation involves using both observation data and underlying dynamics to estimate the hid-

den state of a system. This estimate is presented as a probability distribution. The ensemble Kalman filter (EnKF) utilizes an ensemble of particles to represent the distribution and incorporates observation data through minimum variance estimation. The EnKF has a simple stochastic version known as the perturbed observation (PO) method, but the deterministic version, known as the ETKF, performs better with a small ensemble size. Therefore, the ETKF is a valuable algorithm for practical use. However, the mathematical analysis of the ETKF is more complex than that of the PO method due to its elaborate linear transformation. While previous studies have analyzed the error of the PO method, it still needs to be done for the ETKF. Our study rigorously analyzes the error of the ETKF using an abstract dynamical model that includes the Lorenz system and two-dimensional Navier-Stokes equations on a torus. It's important to note that our setting contains infinite-dimensional dynamics, which adds to the difficulty of mathematical analysis.

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PP1

Distribution-Free Uncertainty Quantification for the Regression Function of Binary Classification

On the poster we present a data-driven framework to construct non-asymptotically exact confidence regions for the true regression function of binary classification. The core idea of this method is to generate alternative outputs based on the conditional distribution that is determined by the candidate function and test whether the alternatively generated datasets are similar to the original sample or not. We give distribution-free, exact, finite sample guarantees regarding the coverage probability of the confidence regions and present sufficient conditions for uniform consistency. The sizes of the confidence regions are also bounded with probably approximately correct inequalities for sample sizes that are large enough. Our theoretical results are validated on illustrative experiments.

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PP1

How to Trust Your Diffusion Model: A Convex Optimization Approach to Conformal Risk Control

Diffusion models hold great potential in solving inverse problems stochastically because they can generate varied and high-quality images. In high-stakes scenarios, such as medical imaging, it is paramount to quantify a model's uncertainty. Has the model hallucinated parts of a patient's anatomy? In this talk, we deploy conformal prediction and conformal risk control to answer two questions: (1) concentration of the samples on the same input, and (2) distance between the samples and the unknown ground-truth image. Denote x, y the ground-truth and degraded images, and $Q_y \approx p(x \mid y)$ the conditional samples from a diffusion model on the same y. We first show that the $\alpha/2$ and $1 - \alpha/2$ calibrated empirical quantiles of Q_y provide entrywise coverage of future samples. Further, we introduce K-RCPS: a novel high-dimensional extension of the Risk Controlling Prediction Sets (RCPS) procedure which guarantees the expected portion of ground-truth pixels not in their uncertainty intervals is below ϵ w.h.p over $(x, y) \sim D$, while minimizing the mean interval length. To do so, we: (1) provably extend RCPS to a high-dimensional, constrained, non-convex optimization problem, then (2) relax the original problem to a convex one to solve it efficiently, and finally (3) devise a statistically-valid procedure to control risk and minimize mean interval length. K-RCPS provides state-of-the-art performance compared to uncertainty quantification baselines.

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Quantum Nv Diamond Spectroscopy

We construct a statistical model for NV spectroscopy and use it in synthetic experiments to solve inverse problems. Our principal application is to develop a primary sensor based on the NV diamond quantum optical properties. This is a significant challenge because the NV diamond structure is sensitive to temperature and pressure as well as magnetic and electric fields, including electromagnetic fields of nearby atoms and molecules. First, using the Hamiltonian for the effects of local strain and the environmental variables, we identify the observable components based on the invertibility of various observation systems. Next, we observe the influence of temperature and pressure on the NV center by solving the Schrdinger Equation and computing the theoretical spectroscopy curve. We assume that the observed photon counts are Poisson random variables with rates proportional to the theoretical spectroscopy. Then, using the Maximum Likelihood Estimation we find the parameter values that maximize the likelihood. Last but not the least we determine the robustness of the model using sensitivity analysis.

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PP1

Drivers of Global Irrigation Expansion Using a Non-Parametric Statistical Modelling Approach:

The Role of Discrete Global Grid Choice

Global irrigation modeling relies on geospatial data and traditionally adopts a discrete global grid based on longitude-latitude reference. However, this system introduces area distortion leading to biased results. We propose using the ISEA3H geodesic grid based on hexagonal cells. To understand the impact of grid choice, we employ a non-parametric statistical framework, utilizing random forest methods, to identify main drivers of historical global irrigation expansion. Irrigation is critical for food security amidst growing population, changing consumption patterns, and climate change. It boosts crop yields, but also alters the natural water cycle and water resources. Understanding past irrigation expansion and its drivers is vital for resource assessment and predicting future trends. We compare the predictive accuracy, the simulated irrigation patterns and identification of drivers between the two grid choices. Results show that using the ISEA3H geodesic grid increases the predictive accuracy by 29%. The model identifies population density, potential productivity increase, evaporation, precipitation, and water discharge as key drivers of historical global irrigation expansion. GDP per capita also shows minimal influence. We conclude that the geodesic discrete global grid enhancing statistical modeling, warranting further exploration in future research across related fields. This analysis lays the foundation for comprehending historical global irrigation expansion.

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PP1

A Measure of Decision-Based Payoff Uncertainty

Based on an observed sample of decisions and their nonnegative payoffs, we isolate a state variable and derive an ex-post optimal payoff sample with respect to the available action sets. The implied relative payoff distribution, on its natural support in [0,1], is the basis for our decision-based payoff (DBP) uncertainty which can take values between 0 and 1. A DBP uncertainty of 0 is measured if an optimal payoff, albeit possibly ex-ante random, has always been achieved in the sample. On the other hand, a maximum DBP uncertainty of 1 obtains when the observed payoff vanishes although a positive payoff could have always been achieved. The DBP uncertainty is compatible with second-order stochastic dominance. It allows for straightforward comparisons between all possible decision problems that feature nonnegative payoffs. The DBP uncertainty is bounded from below by relative regret and therefore links to the framework of relative robust decisions by Weber (Theory and Decision 94(1):3562, 2023). The DBP uncertainty increases in decision complexity, and it vanishes for degenerate choice problems where action sets are mere singletons, in that case irrespective of the observed payoffs. A numerical example concerning the pricing of a product with unknown demand function illustrates the concept.

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Combining the Transport of Intensity and Transport of Phase Equations for Phase Retrieval

We investigate the problem of phase retrieval via the transport of intensity equation (TIE) and transport of phase equation (TPE). The TIE is derived from the paraxial wave equation, together with the TPE, which is usually neglected as, contrary to the TIE, it is nonlinear and also requires information that is harder to acquire than what is required for the TIE. Until now, the TIE has been utilised for phase retrieval problems, although a discussion on the boundary conditions has often been neglected. With this in mind, we provide a discussion of boundary conditions for the TIE. Moreover, the often neglected TPE is also solved and yields boundary conditions which can be applied to the TIE. In our pursuit of solutions for both the TIE and the TPE, we employ the Ensemble Kalman Inversion (EKI) method. As the TPE shares underlying principles with the TIE, our study extends to assess the potential convergence behavior of EKI when applied to both equations. This aspect of our research is particularly intriguing, as it sheds light on the convergence characteristics of EKI in the context of nonlinear problems.

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Stereographic Barker's MCMC Proposal: Efficiency and Robustness at Your Disposal

We introduce a new family of robust gradient-based MCMC samplers under the framework of Stereographic MCMC (Yang et al., 2022) which maps the original high dimensional problem in Euclidean space onto a sphere. Compared with the existing Stereographic Projection Sampler (SPS) which is of a random-walk Metropolis type algorithm, our new family of samplers is gradient-based using the Barker proposal (Livingstone and Zanella, 2022), which improves SPS in high dimensions and is robust to tuning. Meanwhile, the proposed algorithms enjoy all the good

properties of SPS, such as uniform ergodicity for a large class of heavy and light-tailed distributions and "blessings of dimensionality'.

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PP1

Deep Learning Approach for the Semiclassical Limit of the Schrdinger Equation

This paper introduces an efficient method, employing a neural network and Gaussian wave packet, for simulating the propagation of a localized solution of the Schrdinger equation with a smooth potential near the semiclassical limit. Particularly, multi-scale deep neural networks (MscaleDNNs) demonstrate superior performance compared to traditional fully connected DNNs for addressing this specific problem. Explanation and presentation of numerical results are provided to verify. Not only is the computation of an accurate solution our concern, but also the acquisition of an operator mapping an initial value to a solution for this special Schrdinger equation.

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