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IP1

Image Based Modelling of Plant-Soil Interaction

We rely on soil to support the crops on which we depend. Less obviously we also rely on soil for a host of 'free services' from which we benefit. For example, soil buffers the hydrological system greatly reducing the risk of flooding after heavy rain; soil contains very large quantities of carbon, which would otherwise be released into the atmosphere where it would contribute to climate change. Given its importance it is not surprising that soil, especially its interaction with plant roots, has been a focus of many researchers. However the complex and opaque nature of soil has always made it a difficult medium to study. In this talk I will show how we can build a state of the art image based model of the physical and chemical properties of soil and soil-root interactions, i.e., a quantitative, model of the rhizosphere based on fundamental scientific laws. This will be realised by a combination of innovative, data rich fusion of structural and chemical imaging methods, integration of experimental efforts to both support and challenge modelling capabilities at the scale of underpinning bio-physical processes, and application of mathematically sound homogenisation/scale-up techniques to translate knowledge from rhizosphere to field scale. The specific science questions I will address with these techniques are: (1) how does the soil around the root, the rhizosphere, function and influence the soil ecosystems at multiple scales, (2) what is the role of root- soil interface micro morphology on plant nutrient uptake, and (3) how to translate this knowledge from the single root scale to root system, field and ecosystem scale in order to predict how the climate change, different soil management strategies and plant breeding will influence the soil fertility.

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IP2

Differentiable Simulators: Implications for Software Development and Applications to Reduced-order and Data-driven Modelling

Differentiable programming is a programming paradigm that uses automatic differentiation to differentiate a numerical computer program with respect to a set of input parameters, giving gradients that tell us how one should change the input parameters to provide a change in an output state. These can then be used for gradient-based optimization of parameters in the program to match an observed response. Differentiable programming is widely used in frameworks for deep learning like TensorFlow, Theaon, and PyTorch. In this talk, I will outline how one can use differentiable programming to construct fully differentiable simulators for geoenergy applications like CO2 storage, geothermal energy and hydrocarbon recovery. Based on lessons learnt from open-source frameworks like MRST (MATLAB), OPM Flow (C++) and Jutul (Julia), I will discuss how differentiable programming accelerates and improves the correctness of the software development process and aids in the development of efficient nonlinear solvers, e.g., by automatic computation of Jacobians. I also explain how differential simulators can be used as a more physics-true alternative to neural nets and their like in data-driven and reduced-order modelling.

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IP3

Element-based Galerkin Methods in Atmospheric Modeling

In this talk, I will present the role that element-based Galerkin (EBG) methods have had in atmospheric modeling, which includes both climate and weather prediction. I will discuss the strengths and weaknesses of these methods and describe the experiences of my group and collaborators to remedy the identified weaknesses. Among EBG methods, I will describe not only spectral element and discontinuous Galerkin methods, but also flux differencing including kinetic-energy-preserving and entropy-stable methods. I will also touch on the time-integration strategies required for constructing efficient solutions for global, regional, and Large-Eddy-Simulation (LES) modeling and will show results for these regimes. Finally, I will discuss the future of these methods in regards to the changing landscape in high-performance computing and what we need to do to take advantage of exascale hardware. This talk is motivated by my group and collaborators research in building operational weather prediction models as well as advancing the field for application in climate, space weather, and ocean dynamics. A list of publications on these topics can be found at: https://frankgiraldo.wixsite.com/mysite/publications.

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IP4

Remarks and Presentation: A Posteriori Error Estimates Robust with Respect to Nonlinearities and Final Time

A posteriori estimates enable to certify the error committed in a numerical simulation. In particular, the equilibrated flux reconstruction technique yields a guaranteed error upper bound, where the flux, obtained by a local postprocessing, is of independent interest since it is always locally conservative. In this talk, we tailor this methodology to model nonlinear and time-dependent problems to obtain estimates that are robust, i.e., of quality independent of the strength of the nonlinearities and the final time. These estimates include, and build on, common iterative linearization schemes such as Zarantonello, Picard, Newton, or M- and L-ones. We first consider steady problems and conceive two settings: we either augment the energy difference by the discretization error of the current linearization step, or we design iteration-dependent norms that feature weights given by the current iterate. We then turn to unsteady problems. Here we first consider the linear heat equation and finally move to the Richards one, that is doubly nonlinear and exhibits both parabolichyperbolic and parabolicelliptic degeneracies. Robustness with respect to the final time and local efficiency in both time and space are addressed here. Numerical experiments illustrate the theoretical findings all along the presentation.

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IP5

Numerical Methods for Modeling, Editing, and Analyzing Subsurface Structure

Optimized development plans for CO2 sequestration and hydrocarbon recovery require structural models that are geologically realistic and capture subsurface uncertainties. Despite advances in geometric modeling techniques and frameworks for uncertainty quantification, the generation and updating of subsurface models remains a practical challenge. The challenge is even greater when machine learning is used for seismic interpretation due to the vast number of features identified and the presence of false positives. This talk describes numerical methods that address this challenge by supporting automated workflows for structural modeling, editing, and analysis. Our initial focus is on modeling and editing of fault networks with inputs from automated fault detection. Fault surfaces are modeled implicitly using level set methods defined on Cartesian grids. The methodology minimizes surface curvature using a nonlinear least-squares fitting accelerated by multilevel solvers. Semi-automated editing operations support common tasks such as fault extension, projection, truncation, and merging. Once volumetric grids are built, we analyze their structure using a graph-based decomposition into fluid compartments and connections based on the location of spill points and breakovers. The resulting compartment graph facilitates fast evaluation of hydrocarbon charge scenarios and fill patterns for sequestration.

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IP6

Presentation and Closing Remarks: Data Assimilation for Hydrological Predictions in the Subsurface

Predicting water fluxes and water content in the unsaturated zone and recharge into aquifers is challenging due to the lack of information about subsurface structure and the lack of observations. Observations are often local and often give only indirect measures of quantities of interest. Continuous time series of observations can be merged with model predictions to improve predictions over the following time span. The Ensemble Kalman filter is a popular method for data assimilation that is often applied for hydrological predictions. When using it for predictions of water fluxes in the unsaturated zone, uncertainty of parameters and their spatial distribution and model uncertainty are major challenges. A balance between capturing processes in the forward model and dealing with the model error in the data assimilation needs to be found. The talk will discuss methods to deal with parameter uncertainty and unresolved subsurface heterogeneity.

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SP1

SIAM Activity Group on Geosciences Career Prize Lecture: Efficient Global Optimization and Parameter Calibration Involving New RBF Surrogate Algorithms and Application to Global Climate Models and to 3-D Lake Simulations

This talk describes both new global surrogate optimization algorithms for expensive objective functions (including computer simulation models) and their application to specific difficult geophysical problems including calibrating a) large lake 3-D hydrodynamics and water quality ecology model and b) earth system climate models. In some examples one objective function evaluation requires over 5 hours. The mathematical focus is on developing highly efficient general-purpose surrogate global optimization algorithms that can be used for problems with expensive objective functions (possibly with multiple local minima), and black box, like many complex geophysical models. The optimization approach combines a radial basis function (RBF) surrogate approximation of the objective function based on previous objective evaluations and a unique DYCORS method for selecting the next objective evaluation point. All algorithms have a.s. proofs of convergence and include extensions to multi-objective, multi-fidelity and highly parallel algorithms as well as single objective serial algorithms. A major application is to optimize geophysical model parameters to improve the fit to historical data in order to improve model forecasting capability.

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SP2

SIAM Activity Group on Geosciences Early Career Prize Lecture: Scalable Passive Seismology

Over the past decade, new technologies have enabled easier collection of continuous, long-term, broadband seismic data across high-density sensor arrays. Coupled with this, the past two decades have yielded theory and practical guidance to image the subsurface using seismic arrays that record randomly-generated ambient seismic noise. This has yielded many near-surface and environmentally relevant seismic datasets. However, nave algorithms for ambient noise imaging scale poorly with the number of sensors. This talk will present a new set of algorithms for more efficiently tackling ambient noise imaging and improving interactivity of these ambient noise processing workflows.

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CP1

An Efficient Approximation for Multiphase Flow in Complex Subsurface Porous Media

The control volume finite element (CVFE) method is inherently flexible for modelling flow and transport in any geological features often found in the subsurface. The finite element method that captures complex flow characteristics is combined with the control volume approach known for its stability and mass conservative properties. The classical CVFE approach exploits two meshes: the element mesh that represents the material properties element-wise and the control volume mesh, centered on the element vertices, representing the saturation solution in the medium. The discrepancy between those two meshes introduces inconsistency in the transport solution especially along material discontinuities or abrupt material interfaces. In this work, we present an original discontinuous formulation based on the CVFE method for modeling multiphase flow and transport in porous media. We introduce the element pair $P_{1,DG} - P_{0,DG}$ denoting a linear discontinuous Lagrangian velocity approximation and an element-wise pressure approximation, respectively. The formulation enables the use of a single mesh that, in return, does not exhibit the inconsistency issues described earlier. We validate the method and demonstrate the effectiveness of the approach with numerical examples of complex fractures in highly heterogeneous domains.

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CP1

Robust Resolution of Multiphase Chemical Equilibrium Using Parametrization and Cartesian Representation Techniques

The calculation of chemical equilibrium of a multiphase system amounts to finding the quantities of chemical species that minimize the Gibbs free energy under constant temperature and pressure, with mass conservation and non-negativity constraints. This problem can be expressed as the solution of a nonlinear system of equations that presents many numerical difficulties. In particular, Newtons method faces difficulties to converge when one of the species tends to disappear. The remedy usually employed is to work in the logarithm of the concentrations, which improves the situation for small concentrations but significantly degrades the convergence for large ones. The objective of this work is to develop resolution strategies better adapted to these two operating regimes. To do so, we extend to our setting the parametrized form of the switching-variable technique proposed in [K. Brenner, C. Cancs, SIAM J. Numer. Anal., 55 (2017), pp 1760-1785] for the Richards equation. Alternatively, we propose to reformulate the problem by introducing new variables which relax the logarithm of concentrations and whose relation with the concentrations is expressed by a well-balanced Cartesian representation designed to control the partial derivatives. We implement and test these methods on geochemical systems consisting of aqueous, gas and mineral phases at equilibrium. The first results show a clear improvement of the robustness in terms of convergence compared to those of the literature.

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CP1

Efficient Preconditioners for Coupled Stokes-Darcy Problems

Coupled systems of porous media and free flow arise in a variety of applications, such as industrial filtration, blood flow in the human body, and surface/subsurface interactions. For low Reynolds numbers the free flow is governed by the Stokes equations while Darcy's law is used to describe the fluid flow in the porous medium region. The two flow regions are coupled using suitable interface conditions. The discretization of the coupled Stokes-Darcy problem leads to a large, sparse, ill-conditioned, and, depending on the used interface conditions, non-symmetric linear system. To accelerate the convergence of the GMRES method, efficient preconditioners are needed. We focus on preconditioning for the Stokes-Darcy problem discretized by the finite volume method on staggered grids. In this talk, we present three preconditioners and provide spectral as well as field-of-values bounds that are independent of the grid size. Furthermore, we develop inexact versions of the preconditioners that are spectrally equivalent to the exact variants. We illustrate the effectiveness of the preconditioners in numerical experiments.

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CP2

PorePy-Pfc3d FluidSolid Coupling Model with Darcy-Forchheimer Flow Behavior and Its Engineering Application

This study developed a new model, a 3D coupled computational fluid dynamics (CFD)-discrete element method (DEM) model, by coupling two software programs, PorePy and PFC3D, to solve problems related to fluid-solid interaction systems. The Darcy-Forchheimer flow behavior is simulated in PorePy, and the particle migration is simulated in PFC3D. Via Transmission Control Protocol (TCP) socket communication with Python scripting, information between the two software is exchanged in real-time. The classic example in the PFC5.0 documentation was used to verify the model. The PorePy-PFC3D model was employed to simulate the process of water and mud inrush in a water-rich fault tunnel, which could reflect the evolution process of water and mud inrush and track particle movement in a fault zone. The results show that the particles that collapsed inside the fault formed an ellipsoidal distribution during the water and mud inrush in a water-rich fault tunnel. With the continuous loss of particles in the fault into the tunnel, the migration of particles is discontinuous, and a large void appears inside the fault zone. The rapid change of the groundwater flow velocity caused the negative pore pressure. The pressure arch force structure is formed above the ellipsoidal collapse area inside the fault. The principal force field of the fault areas changes from close to the dip of the fault to close to the perpendicular to the fault.

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CP2

Using Elementary Slip Solutions to Solve for Displacement in Complexly Fractured Rock

Geomechanical simulations of fractured rock are challenging and computationally expensive, but indispensable to investigate aperture changes in enhanced geothermal systems (EGS). Since shear displacement due to fluid injection is an especially important mechanism for permeability enhancement in EGS, we focus on fractures subjected to shearing while assuming linear elasticity for the rock matrix. For single fractures with parabolic slip profiles there exist analytical solutions, and due to the linear relationship between maximum slip and induced stress field, these single fracture solutions serve as basis functions in our framework. The total stress field simply is the superposition of the far field- and all slip induced stress fields, while for each fracture the maximum slip value has to be determined based on local force balance constraints. This approach can be refined by abandoning the assumption of parabolic slip profiles and by using an approximation based on a series expansion instead. In any case, however, the number of degrees of freedom can be dramatically reduced as compared with existing mechanical solvers so that more realistic realistic fracture geometries can be handled.

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CP2

Time Series Emulation of Carbon Cycle Model Simulations

Simulators, complex physical models implemented in computer code, are fundamental tools to assess climate change and terrestrial carbon dynamics. Coupled with observational data from satellites, models can infer unobserved ecosystem properties. However, their computational cost typically restricts the number of possible system runs. This limits our understanding of landscapes complex physical processes and associated uncertainties, hindering mitigation and adaptation strategies essential to meet climate change mitigation targets. To facilitate quick model calibration and inference, this work presents statistical methodology to overcome computational constraints by building emulators, or statistical approximations of the simulators. We combined these emulators with history matching to find the set of input combinations for which the simulation gives acceptable matches to observed data. Here, we applied this to the carbon cycle model DALEC Crop, which models the effect of Nitrogen fertilisation on wheat yield in a field over a crop growing season. We applied dimension reduction techniques to emulate Leaf Area Index (LAI) time series and then history matched predictions to Sentinel-2 LAI observations. We then used the input space found in a DALEC Crop forward run to produce plausible yield predictions, skipping DALECs computationally costly model calibration process, to demonstrate the potential to reduce computational costs by using suitable statistical methodology.

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CP2

Torsional Wave Propagation in Functionally Graded Solids with Surface/Interface Energy

The present study investigates the propagation of torsional waves in two models, namely a functionally graded (FG) solid halfspace and two imperfectly bonded FG solid halfspaces considering strain and kinetic energies localized at the surface/interfacece. In order to represent the lack of adhesion between solids, the case of a non-perfect interface is taken into consideration here, i.e. when there is a jump in displacement or in its gradient. The Gurtin-Murdoch (1975) and Eremeyev (2016) approaches are used to derive the surface strain energy density, surface stress tensor, and surface kinetic energy density accounting the non-perfect interface. The dispersion equation for the surface wave have been derived analytically for the two models. A comparative analysis of dispersion curves has been done numerically in order to study effects of FG parameters, surface/interface parameters, and presented by means of graphs. The findings have applications in geosciences and civil engineering for the nondestructive characterisation and study of thin inter-phases between two solids.

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CP2

Smb-Gen: A Bayesian Emulator for Surface Mass Balance Within a Coupled Climate and Ice-Sheet

Computer Model

Asynchronous coupled climate and ice-sheet computer models are used to study atmosphere-ice systems 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 the accumulation of ice 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 with values only returned by the climate model in grid cells where there is a positive surface ice fraction. Each simulation thus yields a different shaped SMB spatial field dependent on the ice fractions returned by the ice-sheet model. 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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CP3

Numerical Method for Compositional Flows on Regular-Lattice Rectangular Porous Network Structures

Simulations of compositional flow involving a gas phase in porous media can be described by a mathematical model. This model includes three types of partial different equations: a hyperbolic equation for the single-phase flow, an elliptic equation for the pressure of the uncompressible flow, and a parabolic equation for the two-phase (gas and liquid) flow. Solving such systems of equations, especially the elliptic equation (pressure solver), can be time-consuming in terms of CPU time. Therefore, we develop a parallel method by using a multi-thread computer structure for solving the pressure equation to speed-up the calculation time. We apply this numerical method to simulate the appearance and disappearance phenomena of compositional flow on 2D and 3D regular-lattice rectangular porous network structures.

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CP3

Adomian Decomposition Method for Shallow Water Waves

Shallow water wave is an important topic in fluid dynamics. A typical example is tsunami caused by earthquakes or undersea volcanic eruptions. There are many disasters in history due to tsunamis which damaged human lives and properties seriously. So it deserves intensive investigation theoretically and numerically in order to understand it deeper. The features of shallow water wave equations are nonlinear second order coupled system of PDEs. Adomian decomposition method (ADM) is employed to solve analytic solutions of this problem. First, for its linearized model we compute a numerical example with periodic solutions, and a symbolic one with unprescribed initial conditions and parameters. The latter is impossibly solved by any numerical method. Both examples are found their explicit exact solutions by ADM. Then we turn to some nonlinear models and obtain their highly accurate approximate solutions. We concluded that ADM is very effective for shallow water wave equations and other nonlinear PDE systems.

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CP3

Step Size Control for Newton and Picard Iteration for the Full-Stokes Equations with Application to Glaciers

Modeling glaciers is computationally expensive. The main computation time is used for solving the full-Stokes equations. Moreover, solving these nonlinear equations is so expensive that simpler equations are used in practice. There exist a Newton and a Picard iteration to solve the full-Stokes equations. We need a step size control for global convergence of Newton's method. Therefore, we minimize a convex functional. This functional has as the directional derivative the variational formulation in divergence-free spaces. The evaluation of this convex functional has nearly no computational costs. If we add a small diffusion term to the equations, we can prove global q-superlinear convergence for Newton's method with Armijo step sizes. The small diffusion term changes the solution only slightly. We compare the Armijo step size for Newton's method with approximately exact step sizes for Newton's method and the Picard iteration. We mean by approximately exact step sizes that we can approximate the exact step size arbitrarily precise but can not calculate it exactly. We test these algorithms with the benchmark experiment ISMIP-HOM *B*, designed by glaciologists to evaluate the quality of ice models.

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CP3

A Study of Tropical Cyclone Intensification Mechanisms Using Large Eddy Simulation and Adaptive

Mesh Refinement

Tropical cyclones (TCs) are responsible for millions of deaths and billions of dollars in damages. Improvements in numerical weather prediction led to improvements of TCs track forecasting. This allows better informed decision making which prevents needless losses. Our ability to predict intensification has also improved, but it still lags compared to improvements in track prediction, since the mechanisms that drive intensification are still somewhat poorly understood. Spectral element simulations at low resolution show that numerical diffusion is able to impact the intensity of both decaying and rapidly intensifying TCs. However, at these resolutions most large scale eddies remain unresolved though they likely affect storm intensity. Large eddy simulation (LES) allows for resolving large scale eddies in a flow and use sub-grid-scale models to model the turbulence of unresolved eddies. LES requires considerably high resolutions in order for results to be accurate. We use a spectral element method and adaptive mesh refinement using p4est to perform LES with a Smagorinsky closure on a TC's inner region, while using a planetary boundary layer scheme away from the core. We analyze the kinetic energy budget by comparing the components of the right hand side of the compressible Navier-Stokes equations, this lets us determine which processes contribute to intensification and which processes hamper it, and how these processes interact at different stages of the TC's evolution.

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CP4

Foam Traveling Wave in Porous Media

Foam injection is an enhanced oil recovery technique with great potential to be applied in Brazilian Pre-salt reservoirs. It consists of injecting gas and surfactant solution in the reservoir to generate bubbles in situ, then reducing the gas mobility, the viscous fingering phenomena, and improving the sweep efficiency. Several papers reported some experimental profiles of water saturations for foam flow in porous media as an unchanging shape profile displacing with time. This evidences the possibility of finding analytical solutions in the form of traveling waves for some foam models. This presentation discusses some traveling wave solutions found for different foam models. We present some traveling wave solutions for a linear kinetic model and show how these solutions qualitatively change for different simplifications in the capillary pressure [Lozano LF, Cedro JB, Zavala RV, Chapiro G. How simplifying capillary effects can affect the traveling wave solution profiles of the foam flow in porous media. International Journal of Non-Linear Mechanics. 2022 Mar 1;139:103867.]. We also adapt this model to include a non-Newtonian foam behavior proposed by Hirasaki and Lawson (1985), and we show in which regimes the analytical solutions for the Newtonian and the non-Newtonian foam models are equivalent [Pereira WD, Chapiro G. Traveling wave solutions for non-Newtonian foam flow in porous media. arXiv preprint arXiv:2209.15134. 2022 Sep 29.].

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CP4

Lightweight Remainder-Based Spatial Refinement Criteria of a Moving Mesh Discontinuous Galerkin Method for 2D Unsteady Convection-Diffusion Problems

In convection-dominated flows, large-scale trends necessarily coexist with small-scale effects. While reducing the convection-dominance by moving the mesh, also called Arbitrary Lagrangian-Eulerian (ALE), already proved efficient, Adaptive Mesh Refinement (AMR) is able to catch the small scale effects. But ALE introduces uncertainties that cannot be neglected compared to the small-scale effects, so that it is unsatisfying to use AMR in an ALE situation in the same way as it is used on static meshes. Consecutively to the study of a remainder-based refinement criterion of a moving-mesh, interior-penalty discontinuous Galerkin (DG) semi-discretization of the 2D nonstationary convection-diffusion equation, we identify which component of the criterion catches the error propagation. This lightweight criterion is then tested and compared to the whole remainder-based criterion.

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CP5

OgsUQ: an Uncertainty Quantification Toolbox for OpenGeoSys

Thermally, mechanically and hydraulically coupled geotechnical applications, formulated in the framework of porous media theory, result in systems of coupled partial differential equations. To solve the discretized version of such a problem, the definition of boundary and initial conditions, as well as all involved parameters, is required. In 3 dimensions, the solution for each unconstrained node of the discretization consists of 5 unknowns for each discretized time point. For uncertainty quantification following problems can be identified: 1.) The number of stochastic input parameters is usually high. 2.) The post-processing result is already large for coarse discretizations. In this contribution, efficient methods, like surrogate modeling and adaptive hierarchical stochastic collocation, for integrating stochastic state spaces with a moderate number of stochastic dimensions are applied to geotechnical engineering. Hereby, it is shown how stochastic post-processing can be performed based on a collection of deterministic finite element post-processing results without further reduction of the data. To enable this, a custom HPC toolbox for OpenGeoSys has been developed in the Julia language, taking advantage of its in-built features, like distributed computing. The framework is demonstrated using an example from radioactive waste disposal in three dimensions.

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CP5

Numerical Modeling of Co_2 Storage: Applications to the FluidFlower Experimental Setup

Carbon capture and storage (CCS) is one of the key technologies that can help industries limit their environmental footprint and societies achieve the climate change mitigation goals. The process entails capturing CO_2 and injecting it into deep geological formations for permanent storage. However, the design and modelling of sequestration projects poses significant technical issues in assessing their risks and consequences. The fate of CO_2 is dictated by many processes including solute transport, multiphase compositional effects, and trapping mechanisms. The ability to properly capture these phenomena is limited by the abstraction of numerical models, the uncertainty in petrophysical characterization, and the modeling of the thermodynamic effects. In this work, we study the impact of each of these factors on the fate of CO_2 storage. We present ensemble-based methodologies to quantify the uncertainties and sample from the posterior. We build on the comparison of the experimental results of the FluidFlower setup and the numerical simulations in IPARS (Integrated Parallel Accurate Reservoir Simulator) to devise recommendations for parameter estimation and modeling assumptions for CO_2 sequestration projects.

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CP5

Improving the Inverse Uncertainty Quantification in Foam-Assisted Enhanced Oil Recovery Using Physically Based Priors

Enhanced Oil Recovery (EOR) models can predict and improve our understanding of multiphase flow in porous media. This work focuses on parameter estimation and uncertainty quantification of the foam flow in porous media. In particular, we present an uncertainty quantification approach based on Bayesian inference to evaluate how different choices of prior distributions affect parameter estimation and propagated uncertainties. Different prior distributions based on physical knowledge and the maximum entropy principle are tested. Our results suggest that the new framework constructed on the physically based priors enhances parameter estimation and uncertainty quantification of the foam flow in porous media.

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CP5

Elastic Functional Changepoint Detection with Application to Merra-2

Detecting changepoints in functional data has become an important problem as interest in monitory of climatologies and other various processing monitoring situations has increased, where the data is functional in nature. The observed data often contains variability in amplitude (y-axis) and phase (x-axis). If not accounted for properly, incorrect changepoints can be detected, as well as underlying mean functions at those changes will be incorrect. In this paper, an elastic functional changepoint method is developed which properly accounts for these types of variability. Additionally, the method can detect amplitude and phase changepoints which current methods in the literature do not, as they focus solely on the amplitude changepoint. This method can easily be implemented using the functions directly, or to ease the computational burden can be computed using functional principal component analysis. We apply the method to both simulated data and two real data sets (MERRA-2 and ERA-5) to show its efficiency in handling data with phase variation with both amplitude and phase changepoints in climate data.

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CP6

Characterization of Different Surfaces Using Fractal Geometry

For the first time in 1983 Mandelbrot introduced Fractal to the world. Fractals are known objects with self-similarity in different scales, i.e., if we look closer at the fractal set, we see a similar geometrical pattern which repeats infinite times to build a fractal object. Mandelbrot fractal geometry could successfully extract mathematical frameworks to model self-similar patterns in nature. The fractal dimension (FD) is a quantitative parameter that has been extensively used to analyze the complexity of structural and functional patterns and it describes a natural object in a better way than Euclidean dimension does. In this study, we will employ the fractal theory to quantify the complexity of different objects in geology. A quantitative analysis commonly known as the Fractal Dimension (FD) analysis has been carried out to illustrate the fractal complexity of these natural examples. Our finding shows that the fractal theory can be used as a mathematical model to further analysis and classification of different real world objects and can be considered as a framework to compare the complexity of these examples and useful tool to differentiate between their patterns.

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CP6

Multiscale Finite Element Method for Shallow Water Equations

Many problems arising from various physical and engineering are multi-scale in nature. Because the presence of small scale and uncertainties in these problems, the direct simulations are prohibitively expensive. Multiscale finite element method (MsFEM) allows to deal with this difficulty. MsFEMs in their classical form have been applied to various porous media problems but the situation in many geoscientific applications with a transport-dominated character is different from porous media applications. In order to study the effect of various parameters like the concentration of pollutants, the dynamics of the background velocity and/or of the temperature in the atmospheric boundary layer, a semi-Lagrangian reconstruction based on multiscale finite element framework (SLMsR) [Simon & Behrens, Semi-Lagrangian Subgrid Reconstruction for Advection-Dominant Multiscale Problems, 2019] for passive tracer transport modeled by an advection-diffusion equation with high contrast oscillatory diffusion was applied. The main scientific contribution of this work will be to extend the multi-scale method to dynamic equation, we will consider the non linear shallow water equations.

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CP6

Physical and Numerical Sub-Grid Modeling with a Particle-Based Approach

Lagrangian particle-tracking methods, free from inherent length scale(s), offer a convenient approach to incorporate micro-scale physics in macroscopic flow and transport models. In stochastic particle approaches, upscaled entities are estimated from the particle ensemble statistics. Further, being impervious to numerical diffusion, particle-based methods are well-suited to capture solution discontinuities. We present a stochastic particle-based framework for multiphase, reactive transport in fractured porous media with a permeable matrix. For solute transport problems, we have previously outlined a conservative particle scheme (in the context of Embedded Discrete Fracture Models) wherein a probability of inter-continuum particle transfer was derived. This scheme has been extended for non-linear hyperbolic transport, relevant to multiphase flow applications [Monga R., Meyer D.W., Jenny P., ECMOR 2022]. To aptly simulate discontinuities, minimal diffusion is added to the system. Thereby, an adaptive diffusion coefficient is proposed, which selectively acts near saturation fronts. We aim to generalize this coefficient for a wide range of flow scenarios. To this end, validation of the particle-based approach, in 2-D settings, with a suitable Eulerian scheme is planned. We envision to model sub-grid processes, e.g., fluid phase-solid matrix interactions, in essence of probabilistic transitions of particles.

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CP6

Multiscale Finite Element Method for Urban Canopies in Climate Models

Canopies represent sub-grid scale features in earth system models and interact as such with the large-scale processes resolved numerically. The canopy is implemented with a viscosity approach, resembling a roughness parameterization. However, the idea is that high viscosity is applied locally to an obstacle area whereas free spaces are assigned low viscosity. In a first step, we test this approach on a micro-scale,using an advection diffusion equation to solve for tracer transport around obstacles. Available wind tunnel data are used for validation of a standard finite element implementation. In a second step, this approach is combined with a multi-scale finite element approach, such that a large-scale simulation can be coupled to the micro- scale representation of a canopy. Comparison of high-resolution standard finite element and low-resolution multi-scale finite element methods will allow for quantitative error analysis. This approach has the potential to lead to better parameterizations of subgrid-scale processes in large-scale simulations.

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CP6

Algebraic Multiscale Grid Coarsening Using Unsupervised Machine Learning for Subsurface Flow Simulation

Subsurface flow simulation is vital for energy storage applications in naturally fractured formations. The challenges posed by the inherent contrasts in geophysical properties have motivated the development of advanced numerical solution methods, such as the Algebraic MultiScale (AMS) solver, which was recently implemented in commercial reservoir simulators. AMS performance is highly sensitive to the basis functions used for restriction and prolongation, which are constructed based on coarse partitions of the physical domain. Simulators typically employ graph-based partitioners to obtain them, which minimize the interfacial area between coarse blocks. This is important to reduce communication between processes, however, it may not be the main consideration for coarse blocks fully contained within a parallel domain. In this work, we propose alternative coarsening algorithms based on unsupervised learning methods, which are attractive due to their direct general applicability. Among them, the Louvain algorithm optimizes partition modularity, while Markov clustering performs random walks to find clusters. Improvement in AMS performance was measured when using these algorithms, compared to a well-known graph-based partitioner, on realistic test cases. While performance results for each algorithm remain case-dependent, these additional options enrich the toolbox available to reservoir engineers aiming to run ensembles of thousands of detailed models.

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CP7

Efficient Adjoint-Based Inversion of Large-Scale Reactive Transport Problem

Gradient-based algorithms are widely used in subsurface inverse problems to estimate unknown parameter fields. It requires the first derivatives (sensitivity coefficients) of the loss function with respect to the adjusted parameters. However, the relation between the unknown parameters and the observations is typically governed by partial differential and nonlinear algebraic equations which makes the gradient very expensive to compute for large-scale problems. This work presents an efficient and elegant approach based on the adjoint state to compute the gradient of the loss function. This approach is implemented in a reactive transport code HYTEC, which is based on a sequential iterative approach (SIA). By construction, solving the adjoint problem requires a corresponding SIA structure. Both spatial and time discretization methods should be considered. The discrete adjoint-state derivation accurately represents the gradient showing more consistent results than the continuous derivation. The developed approach is illustrated on a three-dimensional transient saturated flow-transport problem with mineral oxidative dissolution where observations are heads and concentrations. The adjusted parameters can be porosity, effective diffusion/dispersion coefficients, permeability, as well as species concentrations (mobile and immobile).

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CP7

Bayesian Lagrangian Data Assimilation: Theory and Realistic Applications

Ocean currents and atmospheric winds transport a variety of natural (e.g. aerosols, pathogens, water masses, plankton, sediments, etc.) and artificial (e.g. pollutants, floating debris, search and rescue, etc.) Lagrangian materials. Using dynamically-orthogonal (DO) decompositions, and Gaussian Mixture Model (GMM)-DO filtering, we derive uncertainty prediction and Bayesian learning schemes for both Eulerian and Lagrangian ocean variables in the presence of Lagrangian data. The resulting nonlinear Bayesian data assimilation allows the simultaneous non-Gaussian estimation of Eulerian variables (e.g. velocity, tracers, etc.) and Lagrangian variables (e.g. flowmaps, drifter trajectories, Lagrangian Coherent structures, etc.). We demonstrate the effectiveness of these methods using real data in the Alboran Sea and Gulf of Mexico.

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CP7

Hybrid Newton Method for the Acceleration of Well Event Handling in the Simulation of CO2 Storage Using Supervised Learning

Numerical simulations provide the solution to the multiphase flow equations that model the behavior of the CO2 injection site. However, numerical simulations of fluid flow in porous media are computationally demanding: it can take up to several hours on a HPC cluster to simulate one injection scenario for a large CO2 reservoir if we want to accurately model the complex physical processes involved. This becomes a limiting issue when performing a large number of simulations, e.g. in the process of 'history matching'. During the numerical simulation of CO2 storage in the underground, well events cause important numerical difficulties due to their instant impact on the system. This often forces a drastic reduction of the time step size to be able to solve the non-linear system of equations resulting from the discretization of the continuous mathematical model. However, these specific well events in a simulation are similar across space and time. We propose a methodology to alleviate the impact of well events during the numerical simulation of C02 storage in the underground. We complement the classical numerical algorithm by predicting an initialization of Newton's method directly in the domain of convergence using a supervised learning approach based on recently developed Fourier Neural Operators. Our results show a significant decrease in the number of Newton iterations required for convergence, while ensuring the convergence to the correct solution.

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CP7

Quantum Mechanical Framework for Data Assimilation of Climate Dynamics

An algebraic framework for sequential data assimilation of partially observed dynamical systems is developed. In this framework, the Bayesian formulation of data assimilation is embedded in a non-abelian operator algebra, which provides a representation of observables by multiplication operators and probability densities by density operators (quantum states). In the algebraic approach, the forecast step of data assimilation is represented by a quantum operation induced by the Koopman operator of the dynamical system. Moreover, the analysis step is described by a quantum effect, which generalizes the Bayesian observational update rule. Projecting this formulation to finite-dimensional matrix algebras leads to new computational data assimilation schemes that are automatically positivity-preserving. These methods have a consistent data-driven implementation using kernel methods for machine learning. Moreover, they are natural candidates for implementation quantum computers. Applications to data assimilation of the Lorenz 96 multiscale system and the El Nio Southern Oscillation in a climate model show promising results in terms of forecast skill and uncertainty quantification.

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CP7

An Enhanced Ensemble Smoothing Scheme for History Matching with Unknown Observation Error Covariance

Ensemble-based smoothers are popular data assimilation tools in reservoir applications, including history matching and geophysical inversion. The implementation of such smoothers requires the knowledge of the observation error covariance, which determines the weighting of the observations in the objective function for best estimation of the unknown variables of interest. However, the observation error statistics are often poorly known in real applications, and commonly estimated subjectively based on a diagonal structure of the covariance, neglecting the correlations within the observation errors, which may degrade the quality of the estimates. To overcome this problem, we relax the independent errors assumption by considering a non-diagonal covariance structure parameterized by two hyperparameters, the error variance and the correlation length-scale parameters, and estimate them together with the model variables using a hybrid algorithm that combines the variational Bayesian approach with ensemble-based smoothers. The proposed approach is validated with a linear Gaussian model and a nonlinear reservoir flow model. The results show the enhanced performance of the proposed framework by properly accounting for the uncertainty of observations in the history matching process.

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CP7

Two-Phase Flow with a Data-Driven Flux Model

According to the latest IPCC report, extensive use of CO2 and hydrogen storage is essential to mitigate the climate crisis. When conducting reservoir simulations of these storage techniques, coupled problems are of large interest, as they allow for modeling of composite behavior of two physical processes or the coupling of different models for e.g. near-well and reservoir-scale phenomena. Classically, such phenomena are modeled using physical understanding, expressed in the form of PDEs. In recent years, machine-learning models came into focus that build on experimental data and allow for fast inference. However, iterative methods that solve some sub-problems with classical numerical methods and others with data-driven models, to make use of the respective strengths of both, have not been researched extensively. Here, we introduce a solver for two-phase flow as a model problem for this new approach. Darcy's law is replaced by a data-driven flux model, while the mass balance equation is solved with finite volumes. Due to the unknown nature of the flux model, the elliptic structure of the pressure equation is no longer guaranteed. This affects robustness, as iterative solvers specifically designed for the elliptic-hyperbolic two-phase flow equations may struggle with the modified problem. We investigate how to adjust an iterative solver, such that it still converges to the correct solution. Furthermore, we explore the robustness and computational efficiency of our method.

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CP8

Analytical Solution of the System of Conservation Laws Modeling Foam Displacement WithAdsorption

Motivated by the foam displacement in porous media with linear adsorption, we extended the existing framework for the two-phase flow containing an active tracer described by a non-strictly hyperbolic system of conservation laws. We solved the corresponding Riemann problem by presenting possible wave sequences that composed this solution. We presented necessary and sufficient conditions to guarantee the compatibility of such waves demonstrating the existence of a global solution. We classify the solutions in the phase plane containing all possible left and right states connected by a compatible wave sequence. We point out where the solution is unique and where two different compatible wave sequences exist. We present the CMG-STARS model describing foam displacement in porous media with adsorption and verify that it satisfies the properties necessary for the developed theory. All analytical solutions presented in this model match with direct numerical simulation results.

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CP8

Magneto-Thermoelastic Waves in a Nonlocal Micropolar Orthotropic Solid Half-Space at Impedance Boundary

Purpose The purpose of this paper is to investigate the fluctuation of amplitude ratios of various reflected waves at impedance boundary. Design/methodology/approach The reflection of plane waves on the impedance boundary surface of an orthotropic micropolar-thermo-elastic half-space is investigated in this study with reference to generalized theory of thermo-elasticity for x-z plane. Findings The existence of four coupled quasi plane waves in the plane namely quasi-longitudinal displacement (qCLD) wave, quasi transverse displacement (qCTD) wave, quasi transverse micro-rotational (qCTM) wave and quasi thermal wave (qCT) is proved. From the impedance boundary at $z = 0$, reflection problem of P- wave is studied. The variation of reflection coefficients and energy ratios of various reflected waves is studied. The effects of magnetic field, nonlocal parameters, impedance parameters and angle of incidence are shown graphically on these reflection coefficients and energy ratios. Practical implications The current model can be applied in many different areas, such as soil dynamics, earthquake engineering. In a range of technical and geophysical settings, wave propagation in an orthotropic-micropolar thermoelastic medium with various characteristics, such as initial stress, magnetic field, nonlocality, temperature, etc., gives essential information regarding the presence of new and modified waves. This model may prove useful in modifying earthquake estimates for experimental seismologists, new material designers, and researchers.

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CP9

Metamodeling of Blast Wave Propagation in the Presence of Topography

In this work, the 2D propagation of blast waves in the presence of topography is studied. A high fidelity code resolving the Euler equations is used to obtain accurate evaluations of quantities of interest, e.g. the peak overpressure or the overpressure impulse associated to the blast wave. These outputs are used to predict the potential damages on building. The objective of this work is, with the help of this reference code, to create a metamodel of the propagation, in order to be able to quickly and accurately estimate the outputs with limited computational resources. Many slices of the topography of France are extracted from the database BD Alti and are used as the input of the study. The propagation code is then run for a huge number of topographies and source parameters in order to build a large training dataset. Two methods of metamodeling are considered in this study. First we consider the use of Neural Networks. Different types of architectures are considered such as a multilayer perceptron, convolutional neural networks, or autoencoders. Tensor Train representation is also considered. With this method, the reference code is approximated by a product of order 3 tensors. The metamodels are finally compared on a test dataset where the accuracy and computational efficiency of these methods are estimated and compared.

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CP9

Training Data for Geophysical Inversion

Geophysical inversion is challenging because realistic models of the earth are nonlinear and their corresponding inverse problems are ill-posed due to non-existent or non-unique solutions that are sensitive to small changes in the data. There is now a significant body of work in geophysics that uses neural networks to represent an inverse operator, however, it is difficult to obtain sufficient observational data sets to train a neural network because field data acquisition is both time consuming and costly. Therefore it has become common to create training data with forward

models that capture physical laws, empirically validated rules or other domain expertise. In this work we extend traditional approaches to Bayesian inference to the problem of generating training data from a geophysical forward model. Regularization techniques are used to inform prior information in Bayesian inference which forms the training samples. Unknown hyperparameters in the prior information are found by selecting training samples that pass a χ^2 test. The result is an ensemble of parameter estimates that are propagated through a nonlinear forward model and used as labeled training data in supervised learning. The trained neural network is used to map a set of observations to a set of geophysical parameters.

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CP9

A Critical Appraisal of Kasabov's Can Spiking Neural Networks Predict Earthquakes?"

Kasabov's NeuCube is a spiking neural network framework for learning spatiotemporal brain data. Originally used for integrating brain data modalities such as EEG and fMRI, they posit that it may also be used for non-brain data such as seismological signals. We provide a critical review of these claims, identifying which parts of the NeuCube framework represent biological constraints that may be relaxed when adapting for seismological data. We then discuss source localization problems from neuroscientific imaging and draw a connection to earthquake detection via neuromorphic models for inverse problems on spatiotemporal signals. Finally, we present some results of a reduced NeuCube implementation for seismological data.

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CP9

Computer-Aided Detection of High-Rise Buildings the Curse of Shadows

Due to the increasing global population we observe a worldwide urban sprawl also in those areas previously considered to be too dangerous such as earthquake zones. In case of emergencies a fast survey of damages is vital to efficiently organize rescue operations. Our research is thereby dedicated to automated building detection based on satellite pictures. As this is a pattern recognition problem we apply convolutional neural networks which have proved to be valuable and effective in various scenarios. For regular buildings this method works fairly well. However, regarding high-rise buildings results are far less accurate and our research aims to improve the performance. The reason are adjacent roads as well as building shadows, which especially pose a problem when looking at densely populated areas, i.e. where a large number of high-rise buildings is concentrated on a small area. Besides, having identified the sun as the major influence factor on the performance we propose an alternative identification method based on the solar angle as well as the satellites azimuth and elevation angle. Both algorithms are tested and compared using satellite data from Korea, namely from Sejong and densely populated Seoul area. First results of both methods are promising, however, there is still room for improvement. Current and future work involves the introduction of ensemble learning techniques on the one side and a more refined neural network design on the other side.

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CP9

Fiber Optics Sensors Data Analysis by Machine Learning

Distributed Fibre Sensing (DFS),DAS,DPS,DSS,DTS,FBG,etc sensors are deployed for seismic subsurface data API . The sensing probe of the fiber Bragg grating geophone is made up of Fiber Bragg Gating (FBG).Fiber Bragg Grating Peak Wavelength Detection is done by Wavelet Analysis, discrete wavelet transform (DWT) for the demodulation, demultiplexing and denoising of sensor data, as well as in the detection, extraction and interpretation of measured signal. Singular value decomposition SVD is used for FOS data analysis. Large data set terabyte data analysis is done by machine learning, deep learning ,statistical learning, explainable interpretable machine learning(XML). ANN- time series data analysis-Recurrent Neural Network (RNN),CNN Convolutional Neural Network(images),DNN Deep Neural Network, ResNet Residual Neural Network, unsupervised and supervised machine learning, deep learning, reinforcement learning for seismic imaging and inversion, seismic attributes ,seismic interpretation, reservoir characterization, geosciences data analytics ,bigdata analytics, data assimilation modelling and simulation,etc. Physics Informed Neural Network PINN ,greybox model [whitebox-physics,blackbox-data, black+white= grey], Graph Neural Network GNN machine learning for subsurface imaging and interpretation.FOS data full waveform inversion of seismic data , curvelet seismic wavefield for lithosphere subsurface imaging.

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CP9

Bayesian Data Assimilation and Learning for Coupled Sea Ice-Ocean Systems

Accurate coupled sea ice-ocean models are essential to predict the complex evolution of regional sea ice, and study its impact on climate and navigation. However, numerical models for sea-ice-ocean systems contain various parameters and uncertainties associated with initial conditions, forcing (wind, ocean), and constitutive relations that limit their predictive capabilities. In this work, we develop dynamically-orthogonal (DO) partial differential equation (PDE)-based schemes for sea-ice-ocean probabilistic predictions and use the Gaussian Mixture Model (GMM)-DO filter and neural closure modeling for Bayesian nonlinear data assimilation and learning. Assimilating noisy and sparse measurements, we can then provide probability distributions for uncertain properties of the ice-ocean environment, sea ice velocities, ice height, ice concentrations, ice model parameters, and even ice model formulations themselves. Idealized test cases are showcased, in which we highlight the principled joint nonlinear inference and learning of the coupled ice-ocean state and dynamics.

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CP10

Simulation of Thermo-Poroelasticity Using Enriched Galerkin and Modified Method of Characteristics

We present the mathematical formulation of discretizing thermo-poroelasticity problems by the method of characteristics for the energy balance equation, Enriched-Galerkin for fluid flow, and continuous Galerkin for mechanics. Because of the low thermal conductivities in rocks, the thermal response is dominated by the convection of the fluid flow. Thus, the temperature field has a nonlinear heterogeneity with a sharp-moving front in the case of an injection-production geothermal system. Simulating the energy balance utilizing conventional continuous Galerkin (CG) suffers from grid orientation and numerical dispersion problems and embeds the ability to progress the simulation with large time steps. Therefore, we utilize a modified method of characteristics to model the energy balance PDE that enables large time-stepping without a loss in the simulation accuracy. It also minimizes the overshooting difficulties at the sharp interfaces compared to the CG discretization scheme. The mass balance PDE is solved with the Enriched Galerkin (EG) scheme to ensure the local mass conservation of the pressure field with minimal computational cost. The EG scheme is developed by enriching the CG scheme with piecewise discontinuous constants. Numerical results on various analytical and experimental thermo-poroelasticity problems show matching results, reduced effects of numerical dispersion, front overshoot, and minimal energy and mass balance errors.

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CP10

Scalable Time-Stepping for Nonlinear PDEs Through Krylov Subspace Spectral Methods

Exponential integrators provide an efficient approach to solving large stiff systems of ODEs derived from PDEs, compared to standard time-stepping schemes. However, the bulk of the computational effort in these methods is due to products of matrix functions and vectors, which can become very costly at high resolution due to an increase in the number of Krylov projection steps needed to maintain accuracy. In this talk, exponential integrators are modified by using Krylov subspace spectral (KSS) methods, instead of Krylov projection methods, to compute products of matrix functions and vectors. Numerical experiments, featuring diffusion equations and wave propagation problems, show that this modification causes the number of Krylov projection steps to become bounded independently of the grid size, thus dramatically improving efficiency and scalability. Finally, it is shown how a similar approach can be used to derive multistep methods of Adams type that also realize these benefits.

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CP10

Approximation of Solutions to the Fractional Boundary Value Problems Arising in Geosciences

Fractional calculus is a powerful tool in mathematical modeling, that in the past decades got more attention of applied mathematicians and geoscientists and continues to develop further. Dynamical systems, involving fractional order derivatives, are able to incorporate the so-called memory effects, and due to the non-local nature of fractional differential operators they are usually used in modeling of flows through the porous media (e.g., the groundwater flows), sub- and super-diffusion processes etc. Additionally, a large choice of fractional derivatives and variations in their order give more flexibility in comparison to the classical integer-order models. Since most physical processes are nonlinear and the exact solutions of such models are, in general, impossible to find, we are interested in construction of reliable iterative methods that enable us to deal with this task. In my talk I will present one of such approaches, that is based on analysis of a system of fractional differential equations of the Caputo type, subject to periodic boundary conditions. A proper perturbation of the studied system allows us to reduce analysis of the BVP to an equivalent initial value problem, whose solutions are approximated by coupling the numerical-analytic scheme with Lagrange polynomial interpolation. I will also demonstrate the applicability and effectiveness of this method on a real-world problem.

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CP10

Investigations of Degenerate Equations for Fluid Flow and Reactive Transport in Clogging Porous Media

Structural changes of the pore space and clogging phenomena are inherent to many porous media applications. However, related mathematical investigations remain challenging due to the degeneration of the hydrodynamic parameters. In this research, we apply an appropriate scaling of the unknowns and work with porosity-weighted function spaces. This enables us to prove existence, uniqueness, and non-negativity of weak solutions to a combined flow and transport problem with degenerating, but prescribed porosity field, permeability and diffusion tensor. Moreover, we conduct numerical simulations for the combined, degenerating flow and transport problem. As discretization method, lowest order mixed finite elements are used

and stability of the numerical scheme is shown.

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CP10

A Mixed Finite Element Approach with Error Estimates to a Non-Isothermal Flow Vegetation Model in Porous Media

We consider a vegetation root-soil model which extends the $d = 1$ model originally proposed by Arbogast et al. in 1993 coupling the root and soil models as overlapping continua. Our model in $d > 1$ couples Richards PDE in the soil part and saturated flow in the roots part. We also consider scenarios when the flow depends on soil temperature. A mixed finite element method is applied to obtain numerical solutions of the root-soil system, and we give the proof of the well-posedness for its weak formulation as well as error estimates of the method under some regularity assumptions. We provide numerical examples in 1D and 2D using tomography data of root domains and study convergence errors to validate our theoretical results.

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CP11

ET-MIP: Predicting the Fate and Transport of CO2 in Overburden at the Field Scale

Carbon capture and storage has emerged as a principal emissions reduction technology for the energy transition. Its effectiveness hinges largely on the security of the storage reservoir, which may be susceptible to leakage through permeable pathways such as abandoned wells and faults. Our understanding of the fate of CO_2 in overburden remains limited, hindering the detection and assessment of leaks. There is a need for numerical models capable of accurately predicting the fate and transport of CO_2 in the subsurface. However, continuum multiphase flow models struggle to describe the unstable gas flow regime expected at leak sites. ET-MIP (Electro-thermal macroscopic invasion percolation) couples continuum-based electrical, thermal, groundwater and chemical species modules with a discrete macroscopic invasion percolation gas flow module. It has been validated against bench scale experiments and shown to accurately predict gas behaviour, multiphase transport and capillary trapping all mechanisms which govern the fate of CO_2 in overburden. For application at large-scale field sites however, upscaling techniques will need to be applied to maintain both computational efficiency and predictive capabilities, such that simulation results can inform CO_2 migration mitigation. This talk will first present validation of ET-MIP against a bench-scale CO_2 injection, then outline the upscaling methods applied to move from 2D lab-scale simulations to 3D field scale.

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CP11

Compositional Two-Phase Flow and Phase Behavior in Nanoporous Media: Pore-Level Physics, Pore-Network Modeling, and Upscaling

Fluid flow and transport in porous media often co-occur with phase change dynamics. In a nanometer-scale pore space, the phase behavior of a multicomponent fluid deviates from that in a larger pore space (i.e., micrometer or greater)the pressure and temperature at which the fluid begins to evaporate or condensate in nanopores differ from those in large pores. This pore-size-dependent phase change behavior is further complicated in natural nanoporous media (e.g., clay soil or shale rock) that often contain a significant fraction of interconnected pores spanning from nanometers to micrometers. While the nanoconfined phase behavior in a single nanopore has been extensively studied by molecular-level theories, the new molecular-level understanding has not yet been incorporated in Darcy-scale continuum models. We address this challenge of scale translation by developing a new pore-network-scale modeling framework for flow, transport, and phase change in nanoporous media, which comprises 1) a phase-equilibrium model that accounts for the pore-size and pore-geometry dependent nanoconfinement effects and 2) a fully implicit dynamic pore-network model framework coupling the individual-pore nanoconfined phase-equilibrium model with the two-phase compositional flow. The framework allows one to investigate the interactions between compositional flow dynamics and nanoconfined phase behaviors in complex pore networks and for upscaling phase behaviors to the Darcy-scale.

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CP11

Upscaling of Fluid Flow in Fractured Porous Media

Fractured porous media appear in a large number of applications in nature and industry such as groundwater hydrology, geothermal engeneering, and carbon sequestration. Fractures are narrow heterogeneities with an extreme geometry characterized by a small aperture but wide extent in the remaining directions of space. A common modeling approach is to represent fractures as lower-dimensional interfaces with codimension one. This avoids thin equi-dimensional subdomains that require highly resolved meshes in numerical methods. Given that the flow inside a porous medium is governed by Darcy's law in both bulk and fractures, we derive the limit models in the limit $\varepsilon \to 0$, where ε denotes the characteristic width-to-length ratio of a fracture. The fracture may have a spatially varying permeability and aperture. We assume that the ratio $K_\mathrm{f}^\star / K_\mathrm{b}^\star$ of the characteristic fracture and bulk permeabilities scales with ε^α for a parameter $\alpha \in \mathbb{R}$. Depending on the value of the parameter $\alpha \in \mathbb{R}$, we obtain five different limit models as $\varepsilon \to 0$, for which we present rigorous convergence results. We illustrate our results with numerical experiments.

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CP12

Transition Times of a Particle Driven by Lvy Noise in a Double Well Potential

Inspired by the previous evidence that the DO events can be modelled as transitions driven by Lvy noise, we perform a detailed numerical study of the average transition rate in a double well potential for a Langevin equation driven by Lvy noise. The potential considered has the height and width of the potential barrier as free parameters, which allows to study their influence separately. The results show that there are two different behaviours depending on the noise intensity. For high noise intensity the transitions are dominated by gaussian diffusion and follow Kramers law. When noise intensity decreases the average transition time changes to the expected power law only dependent on the width on the potential and not on the height. Moreover, scaling the equation allows to find a scaling under which the transition time collapses for all heights and widths into a universal curve, only dependent on ??.

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CP12

Monotonicity-Based Methods for Solving Inverse Problems in Linear Elasticity

We deal with the shape reconstruction of inclusions in elastic bodies and solve the corresponding inverse problem by means of monotonicity methods. In doing so, we introduce the rigorously proven theory of the monotonicity-based methods developed for linear elasticity. The key issue of these methods is the Neumann-to-Dirichlet operator and its monotonicity properties. Based on this, we construct the corresponding monotonicity tests. Further on, we take a look at the explicit application of the methods, i.e., the simulation of the reconstruction of inclusions in elastic bodies.

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CP12

The Effect of Plastic Flow on Glacier Dynamics in a Dynamical System Model for Ice Ages

The KCG [Kallen, Crafoord, and Ghil, (1979)] conceptual climate model is a nonlinear DE system which describes the interaction between globally averaged temperature and latitudinal glacier extent. It can be shown to admit the existence of stable periodic solutions in the absence of time-dependent insolation forcing. A key assumption in the reduced model is that the creep law describing glacier flow (strain rate proportional to shear stress to power n) is assumed to be perfectly plastic (limit of infinite n) which reduces the glacier geometry to a parabolic profile [Weertman (1964,1976)]. We revisit the glacier flow model by considering the creep law with realistic creep exponent of finite n. The equilibrium glacier shape and glacier dynamics obtained for finite n have significant differences from the perfect plasticity case. In particular, the steady state glacier shape is determined by a piecewise curve dependent on the creep exponent n and contains a dependence on both surface accumulation and melting. Nonetheless, we show from direct simulation of the PDE for ice sheet dynamics that the ice extent can be described by a first order DE. We then contrast the effect of the creep law exponent for typical ice flow ($n \sim 3$) to the perfectly plastic case ($n \to \infty$) on the prediction of time-periodic oscillations in the coupled dynamical system for ice extent and global temperature.

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CP12

A Nonhydrostatic and Mass Conserving Ground-to-Thermosphere Dynamical Core: Governing Equations and Test Cases

We describe the development of a deep-atmosphere, nonhydrostatic dynamical core (DyCore) targeted towards ground-thermosphere atmospheric prediction. This DyCore is based on a novel formulation of the internal energy equation (IEE), which, unlike standard potential temperature formulations, is valid for variable composition atmospheres. Two versions of an IEE are derived from basic principles. The first version, which uses a product-rule (PR) continuity equation, contains an additional compressible term and does not conserve mass. The second version, which does not use the product-rule (No-PR) in the continuity equation, contains two compressible terms and conserves mass to machine precision regardless of time truncation error. These new equation sets were implemented in two U. S. Navy atmospheric models: the Nonhydrostatic Unified Model for the Atmosphere (NUMA) and the Navy Environmental Prediction System using a Nonhydrostatic Core (NEPTUNE). Numerical results using a deep-atmosphere baroclinic instability, balanced zonal flow, and HA mountain wave experiments are shown. These results are compared to existing deep-atmosphere dynamical cores, indicating that the proposed discretized IEE equation sets are viable next-generation ground-to-thermosphere DyCores. This work was funded by ONR and DARPA.

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CP13

Modeling Evolving Interface(s): Two-Phase & Three-Phase Model Approach

How to describe evolving interfaces? This is a major challenge in formulating a pore-scale model involving such interfaces. It is easy to differentiate between two obvious approaches; namely considering the interface as a sharp transition or as a diffuse transition between the phases. In the case of sharp interfaces, the conservation equations for each phase and the corresponding boundary conditions on the interfaces are implicitly coupled with the equation describing the evolving interface, which makes analysis and implementation troublesome. However, for diffuse-interface approaches, the transition between the phases is considered smooth and of non-zero width. Several approaches to mathematically describe the transition exist, and one such is applying a phase-field variable, which is a smooth phase indicator function approaching, say, 1 in one phase, and 0 in the other phase. The evolving domains and interface are then handled by a phase-field equation; that is, an Allen-Cahn/Cahn-Hilliard equation. Note that the phase-field formulation is on a stationary domain and does not include discontinuities, which makes it more amendable for homogenization and numerical implementations. We will present Allen-Cahn-type phase-field models involving two- and three-phases respectively. We mainly emphasize the major modeling difference between these two models, namely, the triple-point behavior. We will explain the challenges in such models along with some insights.

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CP13

Numerical Analysis of a Hybridized Interior Penalty DG Method for the Cahn-Hilliard System

Diffuse interface models are an increasingly popular approach to the simulation of multiphase flow phenomena. The computational advantage of these models is the elimination of the need to track sharp interfaces between phases, but at the expense of the solution of an additional nonlinear equation arising from thermodynamic considerations. One example is the Cahn–Hilliard equation, which, when coupled to the Navier–Stokes system, can serve as a model for immiscible two-phase flow in porous media at the pore scale. We propose and analyze a hybridized interior penalty discontinuous Galerkin method for the mixed Cahn–Hilliard system wherein additional finite element spaces are introduced on interfaces between mesh elements. By enforcing a suitable transmission condition on the numerical flux, the degrees of freedom on the interior of each element can be eliminated through static condensation. This reduces the size of the globally coupled algebraic system compared to standard DG methods while preserving their many advantages. To ensure unconditional stability of the numerical scheme and unique solvability of the discrete system, we employ a standard convex-concave splitting of the double well potential and an implicit Euler method. We derive optimal a priori error estimates and confirm theory with numerical experiments. If time permits, we will conclude with an exactly divergence-free extension of the numerical scheme to the Cahn–Hilliard–Navier–Stokes system.

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CP13

Study of a Diffuse Interface Model in a Periodic Porous Medium

We consider a diffuse interface model for two and three incompressible immiscible fluid mixture in a porous medium. The system comprises Stokes-Cahn-Hilliard equations coupled via the surface tension term at the micro-scale. We assume that an evolving diffuse interface is present between each pair of the fluids, separating them from one another, having a finite thickness and depending on the scale parameter e. Firstly we derive some a-priori estimates in order to homogenize the model. Using the Galerkins method, we proved the existence of the model in two and three dimensions. We use two-scale convergence and unfolding operator techniques to obtain the desired upscaled model. Further, we derive the corrector estimates to justify the obtained theoretical results. Then, we perform the numerical computations to compare the outcome of the effective model with the heterogeneous micro model.

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CP13

Calcite Precipitation Meets Numerics Preconditioning of a Coupled Cahn-Hilliard Navier-Stokes System

In recent years, much effort has been put into the development of mathematical models for reactive transport in porous media. The models and their theoretical and experimental justification have evolved to more and more complex setups, and less focus has been on efficient numerical techniques to simulate them. This leads to a bottleneck when real-world scenarios are considered. In this talk we focus on precipitation and dissolution effects. We investigate a two-phase flow problem, comprising the Navier-Stokes equations for evaluating the flow field and the Cahn-

Hilliard equation for calculating the evolving diffuse interface between the fluid and solid phases. To solve the discrete, non-linear problem arising from a discretization with finite elements in space and a semi-implicit method in time, Newtons method is applied. A key focus of the talk is the solution of the arising large, sparse and ill-conditioned linear systems. Using problem-adapted and physics-inspired (non-)linear preconditioning, these systems can be solved much more efficiently than by using stock techniques. We discuss both monolithic block-preconditioned approaches as well as partitioned coupling approaches. Furthermore, we present a thorough numerical analysis of our novel schemes.

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CP13

A Phase-Field Model for Subcritical Fracture

We present a new phase-field framework for subcritical fracture in geological materials, in which crack growth occurs at energy release rates below the critical value G_c for a given material. It is assumed that this phenomenon is mainly due to stress corrosion, in which highly stressed material at crack tips is weakened due to chemical reactions in the presence of an environmental agent. Experimental results show that there is a lower threshold of the energy release rate, below which stress-corrosion fracture does not occur. Above this threshold, the speed of crack growth can be related to the crack tip energy release rate via a power relation known as Charles' Law. We incorporate said behavior in a phase-field framework by scaling G_c with a function that varies in time according to the magnitude of a quantity representative of the energy release rate in a regularized fracture setting. No additional field unknowns are introduced relative to the standard phase-field model for fracture, however an ordinary differential equation must be solved to determine the degraded G_c at each material point. We discretize the coupled system via a hybrid formulation that uses finite elements for stress equilibrium and cell-centered finite volumes for the phase-field equation. To assess the performance of the new framework, we perform numerical experiments on both single-crack specimens and more complicated setups involving multiple interacting fractures.

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CP13

Phase Field Modelling for Reactive Transport at Fluid/Solid Interfaces

Modelling reactive porous media is especially complicated if interfaces between different aggregate phases are considered. An example of a recently developed reactive ternary fluid/fluid/solid system is given in [C. Rohde and L. von Wolff. A ternary CahnHilliardNavierStokes model for two-phase flow with precipitation and dissolution. Math. Models Methods Appl. Sci., 31(01):135, 2021], for which we are going to present extensions: First we show, that the CahnHilliardNavierStokes framework can easily be coupled with an ansatz by Wheeler, Boettinger, and McFadden for concentration transport, leading to Rankine-Hugoniot like conditions for the concentration in the leading order of the sharp interface limit. Then, by this coupling it is possible to modify the reaction rate terms, such that arbitrary reactions can be modelled. Furthermore, we discuss different choices of surface tensions. In particular for one specific choice we calculate the sharp interface limit of the model and show that the sharp interface formulation differs from previous results. Then, we develop a non-isothermal description, derive governing equations from the laws of thermodynamics and analyse special cases, e.g. a temperature independent inner energy functional. Finally, we compare this model to existing non-isothermal ones.

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CP14

Adaptive Volcanic Plume Modeling Using Discontinuous Galerkin Methods

Since the Eyjafjallajkull eruption in 2010, the volcanic modeling community has been focused on improving the prediction of ash dispersion and simulation of eruptive columns. While many novel numerical methods have been developed for Computational Fluid Dynamics (CFD) and Atmospheric Modelling, very few have been integrated into models for volcanic erup- tions. Conventional models for plume modeling usually lack high spatial resolution with increasing distance to the volcanic vent which can be an issue for precise estimations of the height of volcanic plumes. Most algorithms for simulating 2D or 3D plumes that are currently available in the volcanic modeling community make use of spatial discretization methods such as Finite Difference (FDM) or Finite Volume (FVM) Methods. Instead of those discretizations, I will present an implementation that is based on the Discontinuous Galerkin Method (DGM) which, additionally, uses Adaptive Mesh Refinement (AMR) techniques to tackle resolution problems and speed up simulations. This implementation of a plume model is based on ? and uses (explicit) Runge-Kutta (SSPRK) methods. With the use of AMR at least 42% of CPU time can be saved while the development of the eruptive column resembles the uniform run qualitatively. We will present results from both uniform and adaptive runs, point out differences, discuss the viability of AMR for the volcanic

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CP14

Numerical Simulation of an Idealized Coupled Ocean-Atmosphere Climate Model

We present numerical simulations for an idealized coupled ocean-atmosphere climate model. Our climate model belongs to the class of intermediate coupled models which are much simpler than the coupled general circulation models of the ocean-atmosphere system but still allow to study the fundamental aspects of ocean-atmosphere interactions. Our model couples an atmosphere system, described by the compressible two-dimensional (2D) Navier-Stokes equations and an advection-diffusion equation for temperature, to an ocean system, given by 2D incompressible Navier-Stokes equations and an advection-diffusion equation for temperature. Finite element method is used to discretize the system of PDEs representing the climate model on a 2D domain and the discrete model is solved using Firedrake, which is an efficient automated finite element method library. To ensure the accuracy of simulation results of the coupled model, we have carried out detailed numerical investigation of its atmosphere and ocean components separately and tested our codes against some benchmark problems available in the literature. Our final goal is to incorporate stochasticity into the coupled ocean-atmosphere model following the Hasselmann's paradigm [Klaus Hasselmann, Stochastic climate models part 1 - theory, 1976] and use the model to study key features of climate phenomena like El-Nino Southern Oscillation (ENSO). This will be the subject of our future work.

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CP14

Coupled Cfd-Mpm Simulation of Submarine Landslides

Material Point Method (MPM) can be used to simulate large deformations in geotechnical problems such as debris flows or landslides. However, simulating the submarine landslides using MPM is quite challenging as it involves complex interactions between debris flow (soil) and seawater (fluid) such as turbulence or hydroplaning mechanisms. This paper presents a coupled Computational Fluid Dynamics and MPM (CFD-MPM) approach to simulate the behaviour of submarine landslides. MPM is employed to model the saturated porous media system, while the CFD is used to simulate the fluid flow by solving the Navier-Stokes equations. The soil - fluid interaction is considered by drag forces in the multi-phase governing equations. We implemented the formulations in the Uintah computational framework. Numerical simulations are performed to highlight the capability of the coupled CFD-MPM model.

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CP14

Explicit Discontinuous Galerkin Method for Surge and Compound Flood Modeling

Recent tropical cyclones, such as Hurricane Harvey (2017), have lead to significant rainfall and resulting runoff with accompanying flooding. When the runoff interacts with storm surge, the resulting floods can be greatly amplified and lead to effects that cannot be modeled by simple superposition of its distinctive sources. Existing numerical models that incorporate both rainfall and riverine flows often consider surrogates to the SWE such as kinematic or diffusive wave approximations. However these are in many cases limited to flows found in inland regions as their assumption are too limiting in coastal regions. Coastal and storm surge models such as ADCIRC, based continuous Galekrin methods may have issues with mass balance due to their conservation properties. On the other hand, shallow water equation (SWE) solvers based on discontinuous Galerkin (DG) methods, avoid these issues due to their local mass conservation property. In this presentation, we present our latest advancements to our discontinuous Galerkin (DG) shallow water equation (SWE) solver as part of ongoing efforts in compound flood modeling for coastal domains. These advancements include rainfall onto the finite element mesh and parametric rainfall models from literature.

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MS1

Room-Scale Carbon Dioxide Injections in a Physical Reservoir Model with Faults

We report a series of physical realizations of room-scale laboratory CO2 injections in faulted geometries in a physical reservoir model. We describe, quantify and discuss key displacement processes, CO2 trapping mechanisms and other relevant parameters for subsurface carbon sequestration including multiphase flows, capillarity, dissolution, and convective mixing. In a room-scale physical model of a subsurface geological cross-section, we perform a series of repeated CO2 injections using the same geometry and identical injection protocols. We describe the degree of reproducibility in CO2 accumulation, multiphase flow patterns and CO2 trapping dynamics with increasing level of geological complexity: i. in a homogeneous trap under an anticline; ii. in a fining upwards sequence; and, iii. In a faulted zone under a fining upwards sequence.

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MS1

The FluidFlower International Benchmark Study: Process, Modeling Results, and Comparison to Experimental Data

Successful deployment of CO2 storage requires an extensive use of reservoir simulators for screening, ranking and optimization of storage sites. However, despite the quarter century since the Utsira/Sleipner injection started, the time-scales of CO2 storage are such that we do not yet have any long-term data set to validate our simulation tools against. As a consequence, we also do not have a basis for assessing the quality with which we can forecast the dynamics of CO2 storage operations. To meet this knowledge gap, we have conducted a major forecasting study for CO2 storage. To achieve reasonable time-scales, a laboratory-size geological storage formation was constructed (the "FluidFlower"), forming the basis for both the experimental and computational work. On one hand, repeated CO2 storage operations were conducted in the FluidFlower, providing what we define as the true physical dynamics for this system (see talk by Fern et al). On the other hand, nine different research groups from around the world provided forecasts, both individually and collaboratively, based on a detailed physical and petrophysical characterization of the FluidFlower sands. Here we report the results of the forecasting study, providing a detailed assessment of the capabilities of reservoir simulators to capture both the injection and post-injection dynamics of the CO2 storage.

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MS1

DarSIA: Darcy Scale Image Analysis Toolbox

In this talk, a newly developed open-source image analysis toolbox is presented. The toolbox is tailored to analyze high-resolution images, such as photographs and PET-CT scans, of porous materials at Darcy scale. Several of its key features will be presented. These include treating images as physical objects, the relationship between image regularization and aggregation of pore-scale information to create Darcy-scale descriptions, tracking of CO2 displacement, and quantifying geometrical deformation due to sand settling. The Darcy Scale Image Analysis Toolbox (DarSIA) has been extensively used to analyze photographs ofmeter-scale CO2 storage experiments conducted in the laboratory FluidFlower rig.

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MS1

FluidFlower Benchmark: Lesson Learned from the Perspective of Subsurface Simulation

In this work, we describe our decisions made to perform the FluidFlower simulation study and discuss various aspects of the benchmark that are different from our usual subsurface simulation practice. We will discuss the impact of various modelling choices to the outcomes of the simulation models, such as gridding, discretization and solver strategies, and the lessons learned, taking into account the different conditions of the FluidFlower study compared to conditions commonly dealt with in subsurface simulation. We will start with a brief description of the DARTS framework utilized for compositional simulation, and the thermodynamic and physical modelling related to the atmospheric CO2-brine system. For the purpose of making meaningful comparisons between each of the modelling choices, we define a baseline model which is a simplified version of the DARTS setup in the main FluidFlower benchmark. The baseline model is then used to study the effect of Cartesian and unstructured meshes, a two-point flux approximation with a multi-point flux approximation and grid resolution on accurate description of the physics at play. Finally, we describe a custom nonlinear solver developed for this benchmark to improve convergence including the linear solver strategy since our default two-stage preconditioner does not perform effectively in this benchmark. We conclude our work with lessons learned and future recommendations.

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MS2

Discontinuous Galerkin Methods for Elliptic and Parabolic Problems with a Line Source

We study interior penalty discontinuous Galerkin (dG) formulations for elliptic and parabolic problems with line sources. For the elliptic problem, we show convergence in global L^2 norms and in broken weighted Sobolev norms. Further, we show that the dG solution converges almost optimally in broken H^1 norms in regions excluding the line. In the L^2 norm, almost optimal local (away from the line) convergence is recovered for linear approximations only and suboptimal rates are shown for high order polynomials. Further, for the parabolic problems, we prove convergence in the $L^2(0,T;L^2(\Omega)$ space for the semidiscrete and a backward Euler fully discrete dG approximations. Numerical experiments for the elliptic problem demonstrate our theoretical findings.

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MS2

Coupled 1D-3D Flow and Transport in Porous Media

The modeling of solute exchanges between an organ and its vasculature is a key component in understanding drug delivery and the treatment of diseases. In this talk, we present a multidimensional model of coupled flow and transport from a network of 1D segments representing the vasculature to the surrounding porous medium representing the organ. The splitting method is applied to the miscible displacement equations.

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MS2

Cellular Traction in Tissues Modelled by Point Sources

Cells exert forces in many circumstances in the (human) body. Examples where cells exert forces are cancer cells that enlarge openings and channels such that they can transmigrate to other parts of the body. Another example is given by muscle cells that exert forces to make joints move. A final example, which we study extensively, is in deep tissue injury, where differentiated skin cells exert forces on their direct environment, which makes the wound contract. Since we are interested in hybrid models where we consider partial differential equations in combination with individual cells that exert forces, we divide the cell boundary into boundary elements on which point forces modelled by Dirac delta distributions are positioned. This approach provides several challenges regarding well-posedness and finite element strategies. During this talk, we will shed some light over these challenges.

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MS2

1D-3D Coupling of Blood Flow Models in Biomedical Applications

We present our work about mixed-dimensional models for simulating blood flow and transport processes in breast tissue and the vascular tree supplying it [1]. These processes are considered to start from the aortic inlet to the capillaries and tissue of the breast. Large variations in biophysical properties and flow conditions exist in this system, necessitating the use of different flow models for different geometries and flow regimes. In total, we consider four different model types. First, a system of 1D nonlinear hyperbolic partial differential equations (PDEs) is considered to simulate blood flow in larger arteries with highly elastic vessel walls. Second, we assign 1D linearized hyperbolic PDEs to model the smaller arteries with stiffer vessel walls. Finally, homogenized 3D porous media models are considered to simulate flow and transport in capillaries and tissue within the breast volume. Sink terms are used to account for the influence of the venous and lymphatic systems. For the 1D-3D coupling, a fourth model is introduced, consisting of ODE systems (0D models). It models the arterioles and peripheral circulation and damps the pressure amplitudes to physiological meaningful values. [1] Fritz, M, Kppl, T, Oden, JT, Wagner, A, Wohlmuth, B, Wu, C. A 1D0D3D coupled model for simulating blood flow and transport processes in breast tissue. Int J Numer Meth Biomed Engng. 2022; 38(7):e3612. doi:10.1002/cnm.3612

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MS3

A Domain Decomposition Method for the Vorticity-Velocity-Pressure Formulation of Stokes Flow

We consider a three-field formulation describing Stokes flow that seeks the vorticity in H(curl), the fluid velocity in H(div), and the pressure in L2. A non-overlapping domain decomposition method is proposed that enforces continuity of tangential vorticity and normal velocity across interfaces with the use of Lagrange multipliers. These multipliers take on the physical interpretation of tangential velocity and pressure, respectively, and we show that the system can be reduced to an interface problem consisting of only these additional variables. To avoid assembly of the reduced system, we employ a Krylov subspace method and discuss functional preconditioners based on the trace regularities of H(curl) and H(div).

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MS3

A Linear Domain Decomposition Method for Reactive Flow in a Porous Medium

We consider a mathematical model for saturated flow and reactive transport in a porous medium. The permeability of the medium is not constant, but depends on the solute concentration. Therefore, the fluid velocity depends on the unknown concentration. On the other hand, the solute is transported by the fluid, so the concentration is dependent on the fluid velocity. An implicit Euler scheme is used for time discretization. This leads to nonlinear, fully coupled time-discrete systems. For solving these systems at each time step, a robust, linear iterative scheme is developed. By adding some linear stabilization terms, one not only makes the scheme linear, but the two components of the model, the flow and the reactive transport of the solute, can be decoupled. Under a mild restriction on the time step, we prove the convergence of the iterative scheme. This convergence holds regardless of the spatial discretization and mesh. This approach is then used to define a linear domain decomposition scheme.

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MS3

Polynomial-Degree-Robust Multilevel and Domain Decomposition Methods with Optimal Step-Sizes for Mixed Finite Element Discretizations of Elliptic Problems

We develop algebraic solvers for linear systems arising from the discretization of second-order elliptic problems by mixed finite elements method of arbitrary polynomial degree, denoted by p. We present a multigrid and a two-level domain decomposition approach in two or three space dimensions. In both cases, our solvers are steered by a posteriori estimators of the algebraic error. We choose the optimal step-sizes by a line search on each level, which allows us to prove that our solvers contract the algebraic error at each iteration, and this for zero pre- and one post-smoothing step only. In both cases, the associated a posteriori estimator is efficient. Importantly, the analysis holds p-robustly in the two-dimensional setting. The proofs require a multilevel stable decomposition of the divergence-free mixed finite element spaces. Numerical results are presented both for the multigrid and the domain decomposition approach and confirm our theoretical findings.

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MS4

Solving Large-Scale Elastic Tomographic Problems

with Source Encoding in the Laplace Domain

Elastic Full Waveform Inversion (FWI) is a state-of-the-art seismic imaging method that provides high-resolution subsurface images and yields additional information compared to purely acoustic approaches. However, an argument against using full-physics wave propagation is that it is computationally expensive. The need for vast computing power to conduct 3-D elastic FWI would seem to prevent its application to 3-D seismic data. Crosstalk-free source encoding remedies the runaway computational cost of full-physics FWI. It reduces the number of seismic sources by forming encoded super-gathers. The main drawback of the source-encoded FWI formulation arises from the difficulty of time windowing the modeled data when inverting only one or a few sparsely sampled frequencies at once. Yet, time windowing would allow for the selection of specific arrivals during the various stages of the inversion, which can effectively mitigate the nonlinearity of FWI. We propose the use of complex-valued frequencies through the Laplace transform for source-encoded FWI, in order to dampen arrivals starting at a given traveltime. In this talk, we will introduce the theory of Laplace-domain source-encoded FWI and demonstrate its effectiveness through numerical tests conducted on challenging seismic datasets collected onshore and offshore.

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MS4

Inverse Problems in Geosciences and Beyond - an Attempt at an Overview

There is a number of inverse problems in Earth sciences with related mathematical structures. Their links are sometimes obvious and in other cases deeply hidden in the mathematical modelling. Also in the latter situation, the exploitation of synergies can become very valuable. This is even the case for transfers of knowledge with medical imaging. Examples of geoscience disciplines with such inverse problems are gravitational field modelling, geomagnetic modelling, and seismic inversions (on large scales). In this talk, a brief overview of some mathematical concepts for such inverse problems is given. This includes the variety of available basis functions as well as approaches for the regularization of ill-posed problems. Reference: V. Michel: Geomathematics - Modelling and Solving Mathematical Problems in Geodesy and Geophysics, Cambridge University Press, Cambridge, 2022.

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MS4

Deep Learning for Reconstruction in Nano CT

Tomographic X-ray imaging on the nano-scale is an important tool to visualise the structure of materials such as alloys or biological tissue. Due to the small scale on which the data acquisition takes place, small perturbances caused by the environment become significant and cause a motion of the object relative to the scanner during the scan. An iterative reconstruction method called RESESOP-Kaczmarz was introduced in [Blanke et al., Inverse problems with inexact forward operator: iterative regularization and application in dynamic imaging] which requires the motion to be estimated. However, since the motion is hard to estimate and its incorporation into the reconstruction process strongly increases the numerical effort, we investigate a learned version of RESESOP-Kaczmarz. Imaging data was programatically simulated to train a deep network which unrolls the iterative image reconstruction of the original algorithm. The network therefore learns the back-projected image after a fixed number of iterations.

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MS4

Global Seismic Tomography with Millions of Waveforms

Recent advances in seismic data acquisition, methodology and computing power have drastically progressed tomographic mod- els. We present global tomography models of 3-D isotropic P-wave velocity in the earths mantle. Multifrequency cross-correlation traveltimes are measured in passbands from 30 s dominant period to the highest frequencies that produce satisfactory fits (3 s). Synthetics up to 1 s dominant period are computed by full wave propagation in a spherically symmetric earth using the spectral-element method AxiSEM. These models are generated using a linear inversion technique in which the traveltime observations are linearly linked to the discretized earth model (as parameterized by an adaptive tetrahedral grid with 400,000 vertices). We discuss the impacts of three factors on the resulting models: (1) data selection; (2) parameterization; and (3) regularization parameters.

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MS5

Towards the Combination of Physical and Data-Driven Forecasts for Earth System Prediction

There is a high degree of interest in applying machine learning to Earth system prediction. It is critical, however, to use physics-informed hybrid methods that combine data-driven models, physical models, and observations. I will present two such hybrid methods: Ensemble Oscillation Correction (EnOC) and the Multi-Model Ensemble Kalman Filter (MM-EnKF). Oscillatory modes in the climate system can be predicted well with statistical methods, often with better skill than dynamical models. However, they only represent a portion of the signal, and a method for beneficially combining them with dynamical forecasts of the full system has not previously been developed. I will show results of applying Ensemble Oscillation Correction (EnOC), a method which corrects oscillatory modes in ensemble forecasts from dynamical models, to forecasts of South Asian monsoon rainfall, outperforming the ECMWF ensemble on subseasonal timescales. A more general method for combining multiple models and observations is Multi-Model Data Assimilation (MM-DA), a generalization of the Kalman filter. Here, I will show how multiple model ensembles can be combined for DA and forecasting in a flow-dependent manner using a Multi-Model Ensemble Kalman Filter (MM-EnKF). This method is applied to chaotic models and results in significant error reductions compared to the best model and to an unweighted multi-model ensemble. Lastly, I will discuss the prospects of using the MM-EnKF for hybrid forecasting.

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MS5

Huge Ensembles (HENS) of Weather Extremes using the Fourier Forecasting Neural Network (FourCastNet)

Studying low-likelihood high-impact extreme weather and climate events in a warming world requires massive ensembles to capture long tails of multi-variate distributions. In combination, it is simply impossible to generate massive ensembles, of say 1000 members, using traditional numerical simulations of climate models at high resolution. We describe how to bring the power of machine learning (ML) to replace traditional numerical simulations for short week-long hindcasts of massive ensembles, where ML has proven to be successful in terms of accuracy and fidelity, at five orders-of-magnitude lower computational cost than numerical methods. Because the ensembles are reproducible to machine precision, ML also provides a data compression mechanism to avoid storing the data produced from massive ensembles. The machine learning algorithm FourCastNet is based on Fourier Neural Operators (FNO) and Transformers, proven to be efficient and powerful in modeling a wide range of chaotic dynamical systems, including turbulent flows and atmospheric dynamics. FourCastNet has already been proven to be highly scalable on NVIDIA-GPU HPC systems. Until today generating 1,000- or 10,000-member ensembles of hindcasts was simply impossible because of prohibitive compute and data storage costs. For the first time, we can now generate such massive ensembles using ML at five orders-of-magnitude less compute than traditional numerical simulations.

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MS5

Towards Ensuring Statistical Climate Reproducibility of Earth System Models in the Exascale Age

Effective utilization of novel hybrid architectures found in near-exascale machines requires code transformations to Earth System Models that may not reproduce the original model solution bit-for-bit. Round-off level differences grow rapidly in these non-linear and chaotic systems, making it difficult to isolate error-growth from the innocuous growth in round-off level differences. Here, we present results from the application of some classical and modern multivariate two sample equality of distribution tests to evaluate statistical reproducibility of atmosphere and ocean model components of Energy Exascale Earth System Model. Baseline simulation ensembles are compared to modified ensembles after a non-b4b change in a model component is introduced to evaluate the null hypothesis that the two ensembles are statistically indistinguishable. To quantify the false negative rates of the tests, we conduct a formal power analysis using resampling methods with targeted suites of short simulation ensembles. Each such suite contains several perturbed ensembles, each with a progressively different climate than the baseline ensemble - obtained by perturbing the magnitude of a single model tuning parameter in a controlled manner. The broad power analyses provides a framework to quantify the degree of differences that can be detected confidently by for a given ensemble size, allowing developers to make an informed decision on an unintentional non-bit-for-bit change to the solution.

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MS5

Ensembles of Ensembles to Support Hierarchies of Purposes

Earth system models are widely used to make multi-decadal projections of climate change. These projections provide both the foundations for much scientific research, and the basis for many societal decisions. Ensembles of simulations with these models provide a route to studying uncertainty in climate projections - a key component of them whatever they are going to be used for. Many questions remain, however, regarding how such ensembles should be designed if they are to provide the most robust information possible in the context of inevitably limited - if nevertheless very large - computational capacity. Here I will introduce the various different types of uncertainty-exploring climate ensembles (forcing ensembles, multi-model ensembles, perturbed-physics ensembles, initial condition ensembles) and reflect on how the characteristics of the different forms of uncertainty lead to radically different targets for ensemble design. The target for initial condition ensembles should perhaps be time-dependent distributions, although model error raises significant mathematical questions regarding the identification of relevant starting conditions. By contrast multi-model and perturbed-physics ensembles require designs which focus on exploring the non-discountable envelope of system response. In both cases generic ensembles are likely to be much less informative than ensembles designed to address specific questions and variables.

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MS6

Pore-Scale Water Retention Behavior in Unsaturated Granular Media Using Multiphase Lattice Boltzmann Method

The Water Retention Curve (WRC) relates matric suction to the degree of saturation degree, and is a fundamental relation for determining the hydro-mechanical behavior of unsaturated soils. Many pore-scale physical phenomena, including hysteresis for drainage and imbibition paths and air entrapment affects the macroscopic water retention. We investigate possible microscopic phenomena that affect the water retention behavior by comparing the liquid/gas phase distributions during drainage and imbibition experiments of granular packings. During imbibition, liquid bridges expand simultaneously to fill pores from smallest to largest, allowing menisci with larger radii of curvature (lower suction). On the other hand, during drainage, only existing gas clusters can expand through the surrounding pore openings, resulting in menisci with smaller radii of curvature (higher suction). We find that the difference in spatial distribution and morphology of gas clusters during drainage and imbibition is the source of hysteresis. Additionally, we also investigate the origin of effective stress from a grain-scale perspective by splitting the forces into suction and surface tension on each grain. We present measurements of the effective stress parameter χ as a function of degree of saturation.

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MS6

Fully-Implicit Sequential Iterative Scheme for Coupled Problems

Flexible numerical tools for pore-scale modelling typically requires to include various multiphysics problems such as the coupled solution of flow, transport, temperature and other fields. In this work, we present a generic framework for dealing with coupled problems in a sequential iterative way. This is particularly convenient when well-established solvers are available for specific sub-problems, but naive sequential solution of each sub-problem do not converge or have slow convergence. We present various examples solved within the OpenFOAM(R) finite-volumes library including a phase-field solver for multiphase flows which involves a fourth-order non-linear Cahn-Hilliard operator which is solved iteratively by the sequential solution of two second-order problems. Other examples include an electrokinetic model based on the Stokes-Nernst-Planck system, as well as simpler linear coupled scalar problems. In this presentation we will focus on the underlying theory of block-coupled differential operators and their solution through block-iterative sequential splitting. We will show various splitting strategies and the need of relaxation terms to stabilise or speed up convergence of the internal iterations.

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MS6

Modeling Coupled Processes in Porous Media Transport Properties Using Direct Simulation and Deep Learning

Coefficients describing transport of momentum, mass, heat or electric current in porous media containing multiple phases are important in hydrology, enhanced oil recovery, energy storage, micro-vascular networks and many other areas. Direct simulation combined with images (e.g. X-ray or scanning electron microscopy) provides a way to compute them in a specific porous medium regardless of its complexity. We present in creating and training predictive deep learning algorithms using direct simulation data that cut down permeability, electrical properties and diffusion coefficients estimation to only seconds. One of the key aspects of machine and learning framework is that it works best with shared (open) data (e.g. Digital Rocks Portal, PI Prodanovic) and open source code. We thus need environments that directly link data, high performance computing simulation, deep learning prediction as well as automated collection of the data into a searchable library.

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MS6

Ostwald Ripening: Bubble Distribution Evolution in Porous Media

Ostwald ripening phenomenon is important for geological gas storage where coarsening can lead to increased mobility of isolated gas bubbles. Gas is typically stored in deep saline aquifers or depleted hydrocarbon fields, representing two-phase and three-phase environments for ripening. We present a chemical-potential based methodology compatible with parallel computations for simulating the ripening of gas ganglia in arbitrary pore geometries. The method is coupled to a conservative level set model for capillary-controlled displacement. The model can assess the impact of isolated oil and water phases in the system and handles real gases. We simulate different fluid distributions and pore geometries in two-phase and three-phase ripening scenarios to study the impact of disconnected liquid phases, gas type, three-phase distributions, and wetting states. The results show that gas solubility and compressibility factor, local capillary pressure, and pore geometry affect the mass transfer rate. In a three-phase scenario, the equilibrium distribution of residual gas bubbles depends strongly on the initial three-phase fluid configuration and its properties (e.g., interfacial tension, wetting state, and interfacial area). In particular, the sizes of bubbles surrounded by oil and water is a function of oil/water capillary pressure. During fluid redistribution, we also identify cases with three-phase double displacements.

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MS7

The Full Drying Process of a Colloidal Suspension: Mathematical Modeling and Numerical Simulations

For a variety of practical applications, it is important to understand the evaporation-induced transformation of a liquid colloidal suspension into a dry porous medium. We present a mathematical model for the full drying process and apply the finite element method to solve it numerically. The relevant phase transitions are directly derived from a reaction-convection-diffusion system for the coupled heat and mass transfer. During the first drying stage, evaporation takes place at the sharp interface between the liquid suspension and the ambient gas phase. The colloids accumulate more and more at the receding interface until they form a porous network strong enough to withstand the evaporation-induced convection. This critical point of time initiates the second drying stage during which the residual water evaporates at a distributed drying front from within the porous medium. Finally, we apply our model to simulate the full drying process of a single droplet taking into account the convection arising from its levitation by a standing ultrasound wave. Empirical data from the literature are used to validate our numerical results.

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MS7

A Two-Scale Phase-Field Model Two-Phase Flow in Porous Media

Two-Phase flow in porous media is relevant for many applications and accurately capturing of interfacial effects in an effective model is central to its modeling. The flow morphology can vary significantly for different physical settings and impact the behaviour on the macro scale. In order to better capture the effects of microscopic interface behaviour on the larger scale, we determine effective parameters from pore-sacle information instead of relying on relative permeability curves. We use phase-fields to model two-phase flow on the pore scale with an advective Allen-Cahn formulation coupled to a Navier-Stokes equation. Using periodic homogenization we arrive at macroscopic equations and microscopic cell-problems that yield effective parameters. Through numerical experiments we investigate the effects of saturations and pore-scale fluid morphologies on the computed tensors. We implement our phase-field model for two-phase flow in DuMu^{X}, using a finite volume discretization. It features staggered control volumes and a combination of cell- and facecentered variables, which communicate using a multidomain coupling manager. This serves as a solver for cell-problems in the two-scale formulation that results from upscaling.

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MS7

Homogenisation of an Advection–Reaction–Diffusion Process in a Porous Medium with Coupled Evolving Microstructure

Many processes in geosciences take place in porous media and cause a change of the microstructure, e.g. sedimentation and dissolution processes. This evolution often depends on a transported concentration and affects strongly the effective permeability. We model such processes with an advection–reaction–diffusion equation which is coupled to Stokes flow and a free boundary on the microscale. In order to derive mathematically an effective model, we transform the problem into a substitute problem on a periodic substitute domain. Thereby, the equations become highly non-linear. Nevertheless, we can homogenise this problem rigorously and obtain an effective model after a back-transformation. It includes an advection–reaction–diffusion equation coupled with a Darcy law for evolving microstructure. Furthermore, the concentration is coupled with the domain evolution via an internal variable and a reference cell in the homogenisation limit. The effective diffusivity becomes time- and space-dependent and can be computed using the solutions of the corresponding cell problems.

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MS8

Geo-Mechanics of Cyclic Loading Relevant for Underground Hydrogen Storage

Underground hydrogen storage (UHS) is a technology which allows for storage of renewable energy in TWh scales. Depending on the geology and energy production geography and scale, one may consider salt caverns or porous reservoirs for UHS deployment. In both types of the reservoirs, the hydrogen is cyclically stored and produced to maintain the continuous supply of energy in the grid. This would mean the pore-pressure (or cavern's pressure) will undergo cyclic low-high values, which then impacts the state-of-the-stress and deformation of the embedding reservoir rock. In this study, we present a generic multiscale approach to benchmark finite elements with lab data, and then run reservoir-scale simulations to quantify the impact of elastic and plastic deformations under cyclic loading. We also validate our approach against real-field measured data from one of the Dutch gas storage sites.

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MS8

Splitting Schemes in Poroelastodynamics and Their Stability Analysis

We study splitting schemes for poroelastodynamics, which can potentially be applied to seismic wave propagation induced by fluid injection such as hydraulic fracturing or fault slip. The fixed stress scheme used in poroelastostatics is first applied to poroelastodynamics. To estimate its numerical stability we perform the von Neumann stability analysis, from which simple application of the fixed stress method does not guarantee unconditional stability in poroelastodynamics because of the second order time derivative term in the wave equation. Thus, we modify the stabilization term of the fixed stress method in order to ensure stability, adding the wave of speed or the Courant number to the stabilization term. From the von Neumann stability analysis, this modified stabilization in the fixed stress method can provide numerical stability. From numerical tests, we find that the a priori stability estimates are supported by numerical results. The modified fixed stress method provides numerical stability with a whole range of time step sizes while the fixed stress method of poroelastostatics might cause instability within some range of time step sizes. Also, the modified fixed stress method reproduces the results of poroelastostatics when the time step size is huge. We will further discuss the pros and cons of the fixed stress and undrained split methods in poroelastodynamics as well as matrix splitting or sequential type preconditioning schemes in the fully implicit method.

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MS8

Mixed-Dimensional Flow Modeling and Upscaling in Fracture Corridors, Joint Swarms, and Fault Zones Incorporating Geomechanical Effects

We present a new methodology to compute stress-sensitive equivalent permeability and transmissibility in complex discontinuity zones (e.g. faults), populated by several geological anomalies with high aspect ratios, such as fractures with infilling, joints, and deformation bands. We explore the nonlinear hyperbolic Barton and Bandis constitutive law between fracture normal stress and aperture in conjunction with a flow-based upscaling method to predict, in an accurate fashion, the magnitude of transmissibility multipliers subject to geomechanical coupling.

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MS8

On Splitting Schemes for Poromechanics

In this work we will focus on splitting solvers for poromechanics. We will first briefly review the main splitting schemes for the quasi-static, linear Biot model and then consider model extensions. This will include nonlinear poromechanics, soft tissue poromechanics and fully dynamic poromechanics. Splitting schemes will be presented. Their convergence, optimization and acceleration will be discussed. Illustrative numerical examples will be included.

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MS9

Physics-Based Machine Learning to Enable Large-Scale Multi-Physics Applications

Obtaining information about subsurface processes is essential to understand the distribution of resources in the subsurface, which is important to address challenges such as providing renewable energy sources. However, the physical processes in the subsurface are high-dimensional coupled processes. The high dimensionality arises for the spatial and temporal domain as well as the heterogeneous distribution of material properties. This yields a computationally expensive model, which makes it often prohibitive to perform global sensitivity analyses or uncertainty quantification. These methods are important to understand which parameters and or processes dominate the state response and how much variability in the solutions we have to account for. In order to address this computational challenge, it is a common procedure to construct surrogate models with and without using machine learning techniques. In this work, we use the non-intrusive reduced basis method, a physics-based machine learning technique, to construct surrogate models that preserve the physical characteristics of the model. Through several case studies, we demonstrate how this can be used to perform probabilistic analysis to gain new insights. Furthermore, we illustrate which requirements need to be fulfilled to construct reliable surrogate models and explain the main difference to other physics-based machine learning techniques such as physics-informed neural networks.

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MS9

Physics Informed Machine Learning for Complex Flows Problems

We present Physics-Informed Neural Network simulations of viscoelastic fluid flow problems. Viscoelastic fluid flow modeling is important in many industrial and medical applications from enhanced oil recovery to blood flow in arteries and polymer processing. The behaviour of those non-newtonian flows is complex and requires a careful treatment of the physical processes involved as well as accurate and efficient numerical techniques. Simulation of such problem class becomes quite challenging when the amount of fluid elasticity is highly increased. This phenomenon is known as the High Weissenberg Number problem (HWNP). Recently, Raissi et al. [M Raissi, P Perdikaris, GE Karniadakis- Journal of Computational physics, 2019 - Elsevier], demonstrated that it is possible to combine Machine Learning approaches with more traditional physics approaches. These so-called physics informed machine learning (PINN) approaches are designed to obtain solutions of general nonlinear PDEs, and they may be a promising alternative to traditional numerical methods for solving PDEs, such as finite difference and finite elements methods. Thus, following this approach we introduce here a framework where we explicitly embed physical laws aiming at describing viscoelastic fluid flow (e.g., Oldroyd/FENEP equations) to constrain neural networks for training a reliable model.

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MS9

PoroTwin: A Digital Twin for a Meter-Scale Porous Media

We present a framework for integrated experiments and simulations of tracer transport in heterogeneous porous media using digital twin technology. The physical asset in our setup is a meter-scale FluidFlower rig. The digital twin consists of a traditional physics-based forward simulation tool and a correction technique which compensates for mismatches between simulation results and observations. The latter augments the range of the physics-based simulation and allows us to bridge the gap between simulation and experiments in a quantitative sense. We describe the setup of the physical and digital twin, including a server-client model for data transfer protocols using cloud technology. The accuracy of the digital twin is demonstrated on a case with artificially high diffusion that must be compensated by the correction approach, as well as by simulations in geologically complex media. Two-way coupling between the physical and digital twin is established by a control tracer transport by manipulating fluid injection and production in the experimental rig. We also discuss extensions to let the digital twin design experiments to enhance its predictive accuracy, thereby realizing an autonomous porous media.

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MS9

Dynamic Mode Decompositions for Inhomogeneous Transport Problems

Rapid advances in software and hardware development have led to the proliferation of bigger and more complex models. One can argue that the growth in model complexity roughly matches that in computational power, so that our ability to perform high-fidelity physics-based simulations remains unchanged. In other words, high-fidelity simulations are still limited by their high computational costs. Reduced-order models (ROMs) are designed to alleviate this computational burden by learning the key features of the underlying dynamics directly from the high-fidelity models output and/or observational data. Dynamic mode decomposition (DMD) is one such data-driven technique, that constructs ROMs of complex dynamical systems by employing singular value decomposition (SVD). We investigate the ability of an extended DMD (xDMD) algorithm to tackle transport problems described by nonhomogeneous PDEs. This new algorithm combines the salient features of the residual and generalized DMD strategies and is proven to smaller error than the standard DMD algorithm which pursues the computation of the best-fit linear operator to approximate the relationship between time-shifted snapshots in time of the solution. The performance of DMD algorithms is tested in terms of representation and interpolation, focusing on the influence of the truncation rank of the SVD and the number of training data.

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MS10

Inverse Magnetization Problems and Localization Constraints

The inversion of a given magnetic field for its underlying magnetization is a non-unique process. The characterization of non-uniqueness depends on the a-priori assumptions on the magnetization; e.g., the magnetization may be assumed to be volumetric or to be confined to a surface, let us say a sphere (which can be reasonable for global geophysics). In this talk, we focus on the latter case. Such magnetizations can be decomposed into two Hardy components and one divergence-free component. Only one of the Hardy components can be determined uniquely from the given magnetic field, unless we make the additional assumption that the underlying magnetization is locally supported in a subdomain of the sphere. We provide a brief overview on what information can be gained from this additional assumption and we construct specific spherical basis functions suited for computations under such a localization constraint.

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MS10

Linearized Inverse Conductivity Problem: Reconstruction and Lipschitz Stability for Infinite-Dimensional Spaces of Perturbations

The linearized inverse conductivity problem is investigated in a two-dimensional bounded simply connected domain with a smooth enough boundary. After extending the linearized problem for square integrable perturbations, the space of perturbations is orthogonally decomposed and Lipschitz stability, with explicit Lipschitz constants, is proven for each of the infinite-dimensional subspaces. The stability estimates are based on using the Hilbert-Schmidt norm for the Neumann-to-Dirichlet boundary map and its Frchet derivative with respect to the conductivity coefficient. A direct reconstruction method that inductively yields the orthogonal projections of a conductivity coefficient onto the aforementioned subspaces is also devised.

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MS10

A Scalable Interior-Point Methods for PDE-Constrained Inverse and Control Problems Subject to Inequality Constraints

We present a scalable computational method for large-scale inverse problems with PDE and inequality constraints. Such problems are used to learn spatially distributed variables that respect bound constraints and parametrize

PDE-based models from unknown or uncertain data. We first briefly overview PDE-constrained optimization and highlight computational challenges of Newton-based solution strategies, such as Krylov-subspace preconditioning of Newton linear systems for problems with inequality constraints. These problems are particularly challenging as their respective first order optimality systems are coupled PDE and nonsmooth complementarity conditions. We propose a Newton interior-point method with a robust filter-line search strategy whose performance is independent of the problem discretizaiton. To solve the interior-point Newton linear systems we use a Krylov-subspace method with a block Gauss-Seidel preconditioner. We prove that the number of Krylov-subspace iterations is independent of both the problem discretization as well as any ill-conditioning due to the inequality constraints. We also present computational results, using MFEM and hypre linear solver packages, on an inverse problem wherein the block Gauss-Seidel preconditioner apply requires only a few scalable algebraic multigrid solves and thus permits the scalable solution of the PDE- and bound-constrained example problem. We conclude with future directions and outlook.

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MS10

Estimating Net Magnetisation of a Bounded Sample from Planar Partial Field Measurements

The process of extraction of relict magnetic information from georocks and meteorites is a challenging task. Due to the weak intensity of the field produced by the remanent magnetisation of a rock, the measurements have to be performed in direct vicinity of the sample and using highly sensitive magnetometric devices such as SQUID and QDM. The basic quantity of interest is the net magnetisation (magnetisation moment vector). Reconstruction of this quantity hinges on effective processing of the experimental data, with the main challenges being the limited measurement area and the noise contamination. Motivated by the concrete experimental settings, I will focus on constructive issues related to asymptotic analysis, field extrapolation and denoising. I will propose and analyse some computational strategies and illustrate their results numerically.

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MS11

Higher-Order Methods for Phase-Resolving Wave/structure Interaction

We consider viscous, inviscid, and depth-averaged models of non-hydrostatic coastal wave propagation over submerged and emergent structures. Our aim is to model wave height attenuation and momentum dissipation through marsh vegetation and over coastal protective structures. Each model requires a significantly different set of numerical methods to achieve higher-order accuracy in a robust manner, and we will discuss several of these, including CutFEM and flux limiting. Finally we present results on experimental data obtained from physical models of wave/structure interaction.

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MS11

High-Order Phase-Resolving Method for Wave Transformation over Natural Shoreline

The use of nature-based facilities, such as mangrove forests, has become a popular solution to coastal hazard mitigation and shoreline stabilization. To reduce the quantification work and uncertain parameterized equations when modeling the wave height attenuation and momentum dissipation through mangrove forests, a new approach for implementing a high order Cut Finite Element Method (CutFEM) for problems of solid structures embedded in multi-phase viscous incompressible flows is presented. This method cuts the fluid meshes to fit the non-conforming embedded solid interfaces so that it allows using the same number of degrees of freedom as the underlying conforming Galerkin method on the fixed background mesh. No explicit generation of cut cell meshes, adaptive quadrature, or local refinement is required. The equivalent polynomials are adopted to compute the exact integration involving products of polynomials with Heaviside and Dirac distributions. Therefore, high-order accuracy for embedded interfaces and robustness of the signed distance representation are gained. The numerical wave elevations show good agreement with the experimental measurements of the wave flume experiment with artificial mangrove forests. The present method can be applied to more complex mangrove system without using any averaged parameters for the embedded structure. All numerical simulations are completed by the open-source toolkit Proteus.

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MS12

Pore-Scale Modelling of Microbially-Enhanced Carbon Mineralization

Large-scale implementation of geological carbon sequestration is considered as a key strategy to limit anthropogenic warming to 1.5 - 2 C, as set out in the Paris Agreement. We are interested in a viable alternative represented by injecting CO2 into reactive rock formations, e.g. basalts, to facilitate rapid carbon mineralization, and therefore increase storage security. Our particular interest lies in microbially enhanced carbon mineralization: biological catalysts are utilized to alter reaction rates and further enhance carbon mineralization. In this talk, we propose a mathematical formulation of the coupled flow and biogeochemical reactive transport problem at the pore-scale. The model is based on optimal decoupling of the reactive transport equations into conservative and kinetic components. We then discuss the construction of a suitable discretization scheme, as well as its integration with the geochemistry package PhreeqPy. We conclude by presenting preliminary model validation results for the geochemical problem of basalt dissolution followed by calcite precipitation. Throughout the talk, special emphasis will be put on the challenges associated with the CO2-rock-biomass interactions at sub-pore levels, specifically the changes in porous microstructure as a response to biogeochemical reactions, leading to changes in the dynamics of flow.

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MS12

Sensitivity Analysis of Engineered Injection-Extraction Systems for Groundwater Remediation

Theoretical and numerical studies on Engineered Injection Extraction (EIE) show that such systems can generate transient groundwater flows that increase plume spreading and contaminant degradation. However, this technology has not yet found a wide application at the field scale. Practical applications need to consider the uncertainty of the hydrogeological and hydrogeochemical parameters, as well as the operational specifications of the wells. To study the effect of uncertain input parameters on the performance of these systems, we conduct a sensitivity analysis using the elementary effect method, also known as the Morris method. The EIE system is composed of four wells that operate alternately following an established sequence proven to enhance mixing. We compute the sensitivities on the peak concentration and analyze the sensitivity ranking to determine the most influential model parameters in different scenarios. We perform conservative and reactive transport simulations in four hydraulic conductivity field configurations. In the case of reactive transport, we apply a mixing-controlled instantaneous complete bimolecular reaction. The parameters considered uncertain in our work are the location and the pumping rates of each well, the geometry of the heterogeneous hydraulic conductivity fields, and the values of the hydraulic conductivity.

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MS13

A Sustainable Infrastructure Concept for Improved Accessibility, Reusability, and Archival of Research Software

Research software is an integral part of most research today and it is widely accepted that research software artifacts should be accessible and reproducible. However, the sustainable archival of research software artifacts is an ongoing effort. We identify research software artifacts as snapshots of the current state of research and an integral part of a sustainable cycle of software development, research, and publication. We develop requirements and recommendations to improve the archival, access, and reuse of research software artifacts based on installable, configurable, extensible research software, multi-modal data representations, and sustainable public open-access infrastructure. Research software artifacts can be reused in varying scenarios. To this end, we develop a multi-modal data representation concept supporting multiple reuse scenarios. Examples of research software artifacts that can be viewed as different modes of the same software-based research result are installation-free configurable browser-based apps to containerized environments, descriptions in journal publications and software documentation, or source code with installation instructions. We discuss how the sustainability and reuse of research software are enhanced or enabled by a suitable archive infrastructure. Finally, at the example of a pilot project at the University of Stuttgart, Germany, we outline practical challenges and experiences.

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MS13

Introducing Open CSMP, a Modelling and Simulation Framework Aimed at Revealing Emergent Behaviour in Complex Geologic Systems

Is a C++17 standard-compliant class library implementing numerical methods and data structures for the combined simulation of thermalhydrological (including reactive multiphase flow)mechanicalchemical (THMC) processes. It is designed for complex geologic models, and interfaced with common geomodelling, meshing, and visualisation tools. Governing equations are discretised in space using a collocated finite-element- (FEM) and finite volume (FVM) mesh and operator splitting (FEM for elliptic & parabolic PDEs; FVM for hyperbolic ones). This approach captures the strengths of both methods and is globally and locally conservative. Computational domains can evolve in shape over time, and multi-domain simulations where different physics are modelled in different regions, are supported. Domains can be coupled using a range of schemes and interface conditions, facilitating discrete fracture, fault and well modelling as well as capillary discontinuities and contact mechanics. Open CSMP also contains asynchronous timestepping methods, and implements dynamic mesh modification, facilitating goal-based simulation. It further provides implementations of: Constitutive relationships for THMC processes Equations of state Property modelling

and analysis functionality Open CSMP evolved from the Complex Systems Platform (CSMP++) that underpins a wide variety of simulation programs and over 200 peer-reviewed publications.

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MS13

Multi-Level Structure in Flow Simulation Codes

The high-performance computing environment for numerical reservoir simulation has changed greatly, from the megaflop machines of the 1970s to the petaflop hardware of today. The demand for more realisations of runs with more detail and, in the case of carbon storage work, much longer timescales, still drives a requirement for more processing power. There has been a change from compute-bound to memory-bound architectures and on the software side, a trend towards multi-layered complexity is apparent. Rather than a single scalar code, we now have systems which are massively parallel on clusters, then multi-threaded on chips, and then have SIMD (single instruction multiple data) pipes on a core: a three-level structure, plus a possible attached GPUs (general purpose graphical processors). Codes typically have a three-language structure, with C++ or Fortran at a high level, C at a low level, then CUDA on the GPU. Some ideas to help address this increased level of complexity are discussed, both organisational, in terms of development teams and in terms of software, such as shared kernel fragments between C++ and CUDA code.

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MS13

Combining Differentiable Geological Parameterizations with Process Simulations

Geological models, as 3-D representations of subsurface structures and property distributions, are used in many economic, scientific, and societal decision processes. These models are built on prior assumptions and imperfect information, and they often result from an integration of geological and geophysical data types with varying quality. These aspects result in uncertainties about the predicted subsurface structures and property distributions, which will affect subsequent simulations, which are based on these models. In this presentation, we discuss the requirements to obtain differentiable geological parameterizations and show implementations for both implicit and explicit surface representation approaches. The methods are implemented in open-source software packages and can be linked to process simulations. An open challenge is still the mesh generation step, but for a subset of model types, the information about gradients can be passed to process simulations as an important step towards uncertainty quantification approaches for combined geological modeling and process simulation.

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MS14

Parameter-Robust Algebraic Multigrid Methods for Interface-Coupled Systems

We are interested in reliable simulations of biophysical processes in the brain, such as blood flow and metabolic waste clearance. Modeling those processes results in interface-driven multiphysics problems that can be coupled across dimensions. However, the complexity of the interface coupling often deteriorates the performance of standard methods to finding the numerical solution. Therefore, we derive preconditioners and solution techniques which target specifically such multiphysics problems for order optimal solving performance. We focus on solvers based on algebraic multigrid method with custom smoothers that preserve the coupling information on each coarse level. We prove that, for the two-level setting, we obtain convergence that is independent of the mesh and material parameters. We show parameter robustness and scalability with regards to number of the degrees of freedom of the system. This is demonstrated on several numerical examples on realistic geometries, such as the interaction of the viscous flow of the cerebrospinal fluid with the poroelastic brain tissue (Biot-Stokes equations) or the mixed-dimensional model of flow in vascularized tissue (3D-1D coupled problems).

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MS14

Mixed and Nitsche's Discretizations of Coulomb Frictional Contact Mechanics for Mixed-Dimensional Poromechanical Models

In this work, we address the discretization of single-phase Darcy flows in a fractured and deformable porous medium, including frictional contact between the matrix-fracture interfaces. Fractures are described as a network of planar surfaces leading to the so-called mixed or hybrid-dimensional models. Small displacements and a linear elastic behavior are considered for the matrix. To simulate the coupled model, we employ a Hybrid Finite Volume scheme for the flow and we investigate two different formulations the contact mechanics. First we consider a mixed discretization combining a P2 Finite Element conforming discretization for the mechanical displacement with a face-wise constant Lagrange multipliers on fractures, representing normal and tangential stresses, to discretize the frictional contact conditions [Bonaldi et al, JCP 2022]. Second, we investigate Nitsche's method [Chouly et al 2013] that involves only the displacement variables and therefore do not require any discrete inf-sup condition unlike the mixed methods. Then, the Nitsche's formulation is compared with the mixed formulation. A variant of The Nistche's method is also investigated both theoretically and numerically which is shown to match the mixed formulation with piecewise constant Lagrange multipliers at the limit of large stabilization parameters. We present several numerical test cases to compare both formulations in terms of accuracy and robustness.

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MS14

Multiscale Preconditioning of Microscale Deformation of Fractured Porous Media

The direct numerical simulation (DNS) of elastic deformation of porous materials on pore-scale digitized images requires large systems of linear(ized) equations to be solved. Krylov solvers are key but suffer from slow convergence without a preconditioner. We present a multiscale preconditioner that significantly accelerates DNS, is scalable on parallel machines, and can be non-intrusively applied within existing codes. The preconditioner is an algebraic reinterpretation of a recent pore-level multiscale method (PLMM) proposed by the authors, which combines a global preconditioner with a local smoother to attenuate high- and low-frequency errors simultaneously. A single application of the global preconditioner is shown to yield approximate solutions that are sufficiently accurate for a wide range of applications (e.g., subsurface). Its combination with a smoother enables improving the approximation further. While cracks are assumed to be static, we propose an adaptive strategy to update the preconditioner for evolving-crack problems without affecting the convergence rate. We validate the preconditioner against DNS and test its convergence for different 2D/3D microstructures and crack patterns. The agreement and performance are favorable.

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MS15

Dissipation in Ageostrophic Turbulence from a Submesoscale Resolving Simulation of the North Atlantic

We diagnose dissipation associated with a downscale energy flux of ageostrophic turbulence in a submesoscale resolving simulation of the North Atlantic. Ageostrophic turbulence was shown to transfer energy towards smaller scales in idealized simulations. To which extent this effect is relevant in more realistic simulations is unclear. Therefore, we use a novel configuration of the ICON-O ocean model where the grid resolution is refined to smaller than 600m over a large area of the North Atlantic. In this simulation, we identify ageostrophic submesoscale eddies by their high Rossby number and diagnose the dissipation associated with these eddies. We find that dissipation is strongly enhanced within the upper ocean, within and south of the Gulf Stream front. Attempts are made to develop parameterizations for the ageostrophic downscale energy flux to couple this energy dissipation with other ocean energy reservoirs. Therewith, we aim to obtain a more realistic view of how much energy becaomes available for diapycnal mixing.

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MS15

Coupling of the Ocean and Atmosphere Dynamics with Sea Ice

In this talk, we discuss a recent approach to a coupled atmosphere-sea ice-ocean model. Starting point are recent rigorous analytical results for Hibler's sea ice model. Indeed, it can be shown that Hibler's sea ice equations subject to a regularized version of the viscous-plastic stress tensor admit a unique, global, strong solution for initial data being close to certain equilibrium points. This result is then used to investigate a model coupling the primitive equations describing the atmosphere and the ocean to Hibler's seai ice model. Based on the theory of quasilinear evolution equations, we obtain local well-posedness for this model subject to various coupling conditions.

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MS15

Seamless Scheme for Compressible, Soundproof, and Hydrostatic Dynamics with Applications in Balanced Data Assimilation

This talk will summarize recent developments of a family of semi-implicit finite volume discretizations for atmospheric flows. These schemes are designed to work with uniform efficiency for the full compressible flow equations as well as for various scale-dependent reduced dynamics, as described by the pseudo-incompressible, hydrostatic and quasi-geostrophic models. We discuss the theoretical background of the model family, the design of the discretizations compatible with the respective asymptotic limits. Moreover we present an approach to data assimilation (DA) that avoids the introduction of unphysical imbalances in the DA steps by judiciously utilizing the seamless approximation qualities of the numerical solver.

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MS15

On the (Non-)Uniqueness of Solutions to the Linear Transport Equation

One of the main questions in the theory of the linear transport equation is whether uniqueness of weak solutions to the Cauchy problem holds in the case the given vector field is not smooth. In the talk I will provide an overview on some results obtained in the last few years, showing that even for incompressible, Sobolev (thus quite well- behaved) vector fields, uniqueness of solutions can drastically fail. This result can be seen as a counterpart to DiPerna and Lions well-posedness theorem.

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MS16

Direct Multi-Modal Inversion of Geophysical Logs Using Deep Learning

We present a proof-of-concept approach to multi-modal probabilistic inversion of geophysical logs using a single evaluation of an artificial deep neural network (DNN). A mixture density DNN (MDN) is trained using the multiple-trajectory-prediction loss functions, which avoids mode collapse typical for traditional MDNs, and allows multi-modal prediction ahead of data. The proposed approach is verified on the real-time stratigraphic inversion of gamma-ray and rate-of-penetration logs. The multi-modal predictor outputs several likely inverse solutions/predictions, providing more accurate and realistic solutions than a deterministic regression using a DNN. For these likely stratigraphic curves, the model simultaneously predicts their probabilities, which are implicitly learned from the training geological data. The stratigraphy predictions and their probabilities obtained in milliseconds from the MDN can enable better real-time decisions under geological uncertainties.

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MS16

Ocean-Connected Supermodel of the Earth System

A supermodel connects different models interactively so that their systematic errors compensate to produce a model with superior performance. It differs from the standard non-interactive multi-model ensemble (NI) approach, which combines model outputs a-posteriori. The development of supermodels with state-of-the-art Earth System Models (ESMs) has not been possible because it is technically challenging to combine models that do not share the same state space. Here, we formulate the first supermodel framework for different ESMs and use data assimilation to synchronize models. The ocean of three ESMs is connected every month by assimilating pseudo sea surface temperature (SST) observations generated from a weighted mean of the multi-model on a common grid to handle discrepancies in grid and resolution. The weights are spatially and seasonally varying and estimated using a Bayesian framework from the SST bias of the NI. The supermodel achieves synchronization in the ocean and atmosphere in locations where the ocean drives the climate variability. The time variability of the supermodel multi-model mean SST is reduced compared to the observed variability; the damping is greatest where synchronisation of the atmospheric components is least and is lower-bounded by NI. Supermodel strongly reduces the SST bias and mitigates the double Intertropical Convergence Zone precipitation bias in the tropics.

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MS16

Reconstruction of Arctic Sea Ice Thickness (2000-2010) Based on a Hybrid Machine Learning and Data Assimilation Approach

In the Arctic, the sea ice thickness (SIT) remains one of the most challenging parameters to estimate and generally present temporal and spatial discontinuity which are a major difficulty for climate studies. Since 2010, the combined product CS2SMOS enables more accurate SIT retrievals that significantly decrease the SIT errors when assimilated in models (such as TOPAZ4). Can we extrapolate these benefits in the earlier period 2000-2010? In this study, we train a machine learning (ML) algorithm to learn the systematic SIT errors between two versions of TOPAZ4 (with and without CS2SMOS assimilation) in 2010-2020, in order to predict the SIT error and extrapolate the SIT prior to 2010. The ML algorithm relies on SIT coming from two versions of TOPAZ4, various oceanographic variables as well as atmospheric forcings (from ERA5). The ML model demonstrates its ability to correct a significant part of the SIT error. We will discuss the sensitivity of the method to the input variables and to different types of ML models. The long Arctic ML-reconstructed SIT record (2000-2022) is validated using in-situ data and earlier satellite data.

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MS17

Stochastic Forecast of Extreme Sea-Level Hazards: Framework and Practical Implementation

As they are rare, localized and variable in time, coastal hazards due to extreme sea-levels are known to be difficult to forecast with the deterministic and ensemble approaches presently implemented around the world. An alternative architecture for extreme sea-level early warning systems based on uncertainty quantification and optimization is thus presented. It aims to minimize the numerical cost and calculation time of the near real-time forecasts while maintaining the reliability and trustworthiness of the hazard assessments. It is based on three modular components: (1) a surrogate model (e.g., polynomial chaos expansion, Gaussian processes, machine learning) (2) a fast data assimilation via Bayesian inference and (3) an optimal experimental design of the observational network. The new architecture has been partially implemented in the Adriatic Sea within an early warning system for meteotsunamis tsunami-like ocean waves driven by atmospheric disturbances. It is based on the Adriatic Sea and Coast (AdriSC) modelling suite for the deterministic forecast of the atmospheric conditions at 1.5-km resolution and the barotropic ocean conditions at up to 10 m along the coasts. However, it fully relies on a meteotsunami surrogate model for the hazard assessments at known sensitive locations in Croatia. We will present the advantages and the drawbacks of such an approach through several applications of the AdriSC modelling suite during meteotsunami events.

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MS17

Towards the Incorporation of Compounding Processes in Non-Stationary Probabilistic Tsunami Hazard Assessments

Tides are often the largest source of daily sea levels fluctuations. Two new probabilistic tsunami hazard assessments (PTHA) methods are proposed to combine the tidal phase uncertainty at the moment of tsunami occurrence with other sources of uncertainty. The first method adopts a Stochastic Reduced Order Model (SROM) producing sets of tidal phase samples to be used in tsunami simulations. The second method uses tsunami simulations with prescribed collocation tidal phases and tide probability distributions to model the uncertainty. The methods are extended to non-stationary probabilistic tsunami hazard assessments (nPTHA), combining tsunamis, tides and sea level rise (SLR). As an illustration, these methods are applied for assessing tsunamis generated in the Manila Subduction Zone and impacting the coasts of Kao Hsiung and Hong Kong. While the SROM-based method is faster solving for the studied PTHA if only tides are considered, the collocation-based method is faster when both SLR and tides are considered. The results of the illustration show that tides have a relevant impact on the PTHA. However, the SLR within an exposure time of 100 years has stronger impact. It is perhaps counter-intuitive for the increase in hazard from SLR to be greater than the increase from tides, when the perception by the general public may be that tides are much bigger than estimates of SLR, because of familiarity.

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MS18

Phase-Field Modelling of Evolving Adhesive Interfaces

Computational phase-field modelling is a powerful and versatile mathematical technique to describe and solve problems that involve evolving interfaces. In this contribution, we present a new phase-field model for adhesion and discuss its underlying foundations in terms of thermomechanical consistency. The interaction between adhesive interfaces is modelled by the introduction of a coupling term in the classical free energy. The resulting phase-field model is a stiff, higher-order, non-linear partial differential equation, in which adhesive interaction is regularized onto the moving interfaces. We characterize the singular limit of the adhesion problem. Under the assumption of the existence of a smooth limiting interface, we identify the limiting sharp-interface energy of our adhesion problem and demonstrate that its minimisers are geometric surfaces with a non-trivial adhered part. Lastly, we provide numerical examples of adhesion and show how unconditionally energy-stable results can be obtained by using the scalar auxiliary variable approach as time-discretization scheme. Furthermore, we discuss application of the presented model to problems in cell biology, which is vital in understanding numerous biological processes, including cell migration, structural integrity and signal transduction. We show how the model can be extended to account for the protein dynamics at a cells membrane, which govern the binding and unbinding of a cell to its extracellular environment.

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MS18

Efficient Implementation of a Conservative Phase-Field Model for Evolving Fluid-Solid Interfaces

Mineral precipitation and dissolution in porous media cause changes to the porosity and to the porous structure of the medium. At the pore scale, one therefore has evolving fluid-solid interfaces as solutes leave or join the saturating fluid and the solid mineral phase. This means that at the pore scale, the fluid and solid phases correspond to time-dependent domains. To model the fluid flow and solute transport in such domains, we apply a phase-field model at the pore scale. We here apply an Allen-Cahn model for the fluid-solid interface evolution. The standard Allen-Cahn equation is not conserving the phase-field variable, which can lead to unphysical evolution of the fluid-solid interface. We therefore consider an extended formulation, which includes a non-local term that ensures the Allen-Cahn model to be conservative. However, applying Newtons method to solve the resulting non-linear system of equations is slow due to the presence of the non-local term and we instead apply the L-scheme. The L-scheme iterations are guaranteed to converge, although with only linear convergence. The L-scheme is still more efficient as each iteration is cheaper, and it is robust in terms of initial guess for the iterations. This implementation is hence efficient and robust, and can model mineral precipitation and dissolution in porous media in a conservative manner.

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MS18

Singularities and Surprises in Hele-Shaw and Porous Media Models of Immiscible Two-Phase Displacement Flows Involving Non-Newtonian Fluids

We discuss two specific types of problems. First we consider viscoelastic Hele-Shaw flows involving two immiscible upper convected Maxwell fluids (Journal of Non-Newtonian Fluid Mechanics, 309 (2022) 104923; 303 (2022) 104773) and show that singularities up to three types can occur including resonance and fracture, the latter one consistent with the experimental results of Mora and Manna (J. Non-Newtonian Fluid Mech. 173-174 (2012) 30-39). The resonance occurs when one of these two fluids is air and is removed when air is replaced by a Newtonian fluid. The Oldroyd-B case currently in progress may also be discussed. This is joint work with Zhiying Hai. The second problem we consider is shear-thinning polymer flooding. We discuss a novel framework for incorporating this effect in a surfactant-polymer flooding simulator developed by Daripa and Dutta (J. Comp. Phys. vol. 335, pp. 249-282 (2017)). This framework is data driven and implements the values of power-law coefficients empirically guided by the local values of concentration and shear rate. We demonstrate the importance of such a data-driven model and the potential it holds for improved modeling of polymer flooding to make an informed decision while choosing a polymer for a given flood simulation. Simulation reveals unexpected role of data driven shear thinning effect such as traveling viscosity waves and very mild viscous fingering. Thanks to Rohit Mishra for performing the simulations.

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MS18

An Efficient Coupling of Free Flow and Porous Media Flow Using the Pore-Network Modeling Approach

Macro-scale models of coupled free flow and flow through a permeable medium often lack the capabilities to account for process-relevant complexities on the pore scale. Direct numerical simulation of such systems, on the other hand, inherently includes these micro-scale features but is only feasible for problems of very limited spatial and temporal extent. A new class of hybrid models aims to combine the individual strengths, i.e., computational efficiency and local accuracy on the micro scale, of models of different dimensionality. We will present, a fully coupled model concept that involves a (Navier-)Stokes model for the free flow and a pore-network model for the porous domain. As a first step, we consider isothermal single-phase flow with and without component transport, but the model is open for the extension for more complex physics. Appropriate coupling conditions guarantee the continuity of mass and momentum fluxes across the interface between the two domains. We use a monolithic approach, i.e., all balance equations are assembled into a single system matrix and no coupling iterations between the submodels are required. Newtons method is applied to solve the potentially non-linear system of equations.

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MS19

Some Thoughts on Ensemble Means and the Curse of High Dimensions

Future climate projections rely on high dimensional climate model simulations. With model uncertainties and variations between realizations, outcome from different models are conglomerated and compared. There are even model inter-comparison projects with protocols specifying conditions, to enable direct comparisons and model means. A simple argument tells that the model mean of sets of high dimensional models will perform better in comparison with observations than any of the individual model members. This is contra-intuitive in the sense that one would expect the "best" model to outperform a mean including "lesser" models. I will discuss this issue and wht to do about it.

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MS19

On the Parametric Dependance of Climate Model Errors and Feedbacks

Climate models produce high dimensional output across space, time and variable dimensions. Their calibration is subject to both data, time and computational constraints. Perturbed parameter ensembles (PPE) are ensembles of simulations for which the physical parameters have been perturbed according to a defined sampling. Using a PPE of the CNRM-CM6-1 atmospheric model, we argue that the effective degrees of freedom in model performance response to parameter input is, in fact, relatively small, explaining why manual calibration is often able to find near-optimal solutions. However, there is a potential for comparably performing parameter configurations making different tradeoffs in model errors, with potentially different future climate evolution. Indeed, the uncertainty associated with climate model tuning is rarely represented in climate sensitivity estimates. We propose a quasi-automatic optimization method for selecting a subset of optimal calibrations with a diversity of feedback parameter values. Using a statistical emulation/optimization framework, 15 simulations tuned with different combinations of the 30 parameters values are identified, presenting a score comparable to that of the CFMIP6 multi-models, while covering an estimated ECS interval of [4.1 - 6.1]. These results illustrate the impact of model calibration on a model estimate of ECS, highlighting the importance of better quantifying calibration uncertainty in climate projections.

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MS19

Ensemble Design for Sensitivity Analyses Using the Energy Exascale Earth System Model (E3SM)

This talk will discuss ensemble design for sensitivity analyses using the U.S. Department of Energys Energy Exascale Earth System Model (E3SM). We will present and discuss results from a variance-based global sensitivity analysis (GSA) using a fully-coupled, ultra-low resolution (ULR) configuration of version 1 of the E3SM (E3SMv1), performed as a first step towards quantifying parametric uncertainty in Arctic feedbacks. The study randomly draws 139 realizations of 10 model parameters spanning 3 E3SMv1 components, which are used to generate 75-year long projections of future climate with a fixed pre-industrial forcing. We quantify the sensitivity of 6 Arctic-focused quantities of interest to these parameters using main effect, total effect and Sobol sensitivity indices computed with a Gaussian process (GP) emulator. A sensitivity index-based ranking of model parameters shows that the atmospheric parameters in the CLUBB (Cloud Layers Unified by Binormals) scheme have significant impact on the Arctic climate. We also use our GP emulator to predict the response of varying each variable when the impact of other parameters is averaged out. Our study confirms the necessity of performing global analyses using fully-coupled climate models, and motivates follow-on studies involving the ULR model. Time-permitting, we will present some preliminary work involving ensemble design for a sensitivity study to understand the impacts of Stratospheric Aerosol Injection using the E3SM.

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MS19

Implementation and Verification of ESM-ML Hybrids

Machine Learning (ML) has raised significant interest across many scientific disciplines, and has also attracted Earth system modellers, who are also looking into these methods to improve their models. Particular areas of interest include the use of ML to build better parameterizations for sub-grid processes or to model unknown physics based on observations; using ML for ensemble production and downscaling; or using ML for full model replacement. Since Earth System Models (ESMs) are typically written in parallelized Fortran and ML implementations are relying on a Python-based ecosystem of frameworks, the convergence towards coherent hybrids of ESMs and ML, able to power large-scale computation jobs, poses some technical challenges at the level of interfaces and parallelization, but also raises overarching concerns of software system design including user-friendly build chains and long-term maintenance strategies. Yet, even as these challenges are being addressed, a primary concern remains regarding the scientific validity of such hybrids. ML algorithms act as universal function approximators, and are tuned against large-scale data. While several strategies exist to also incorporate physical knowledge, ML components can easily be perceived as black boxes. Therefore, the validity of ESM-ML should best be assured by scientific validation against standard scenarios that can only be defined by the domain science communities.

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MS20

Geometrically Intrinsic Modeling of 2D Diffusive Wave Overland Flow for Coupled Surface-Subsurface Hydrological Applications

Shallow water models of geophysical flows must be adapted to geometric characteristics in the presence of a general bottom topography with non-negligible slopes and curvatures, such as mountain landscapes. In this paper we derive an intrinsic formulation for the diffusive wave approximation of the shallow water equations, defined on a local reference frame anchored on the bottom surface. We then derive a numerical discretization by means of a Galerkin finite element scheme intrinsically defined on the bottom surface. Simulations on several synthetic test cases show the importance of taking into full consideration the bottom geometry even for relatively mild and slowly varying curvatures.

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MS20

Simulation of Coupled Multiphysics Problems in Large Deformation Regime

Natural hazards involving large mass movements such as landslides, debris flows, and mud flows often cause important damages to our structures and to the surrounding landscape. The numerical simulation of the above events still represents a big challenge mainly for two reasons: the need to deal with large strain regimes and the intrinsic multiphysics nature of such events. While the Finite Element Method (FEM) represents a recognized, well established and widely used technique in many engineering fields, unfortunately it shows some limitation when dealing with problems where large deformation occurs. In the last decades many possible alternatives have been proposed and developed to overcome this drawback, such as the use of the so called particle-based methods. Among these, the Material Point Method (MPM) avoids the problems of mesh tangling while preserving the accuracy of Lagrangian FEM and it is especially suited for non linear problems in solid mechanics and fluid dynamics. The talk will show some recent advances in MPM formulations, presenting both an irreducible and mixed formulation stabilized using variational multiscale techniques, as well as the partitioned strategies to couple MPM with other techniques such as FEM or DEM. All algorithms are implemented within the Kratos-Multiphysics open-source framework and available under the BSD license.

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MS20

A Spectral Method for the Numerical Solution to the Nonlocal Discontinuous Richards' Equation

We propose a spectral method based on Chebyshev polynomials to study a nonlocal derivative free Richards' model derived by the peridynamic formulation of continuum mechanics. We prove the convergence of the semi-discrete scheme and provide several simulations to study the properties of the solutions.

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MS20

Control-Volume Finite-Element Schemes for Coupling Free Flow with Porous-Medium Flow

Exchange processes across a porous-medium free-flow interface occur in a wide range of environmental, technical and bio-mechanical systems. In the course of these processes, flow dynamics in the porous domain and in the free-flow domain exhibit strong coupling, often controlled by mechanisms at the common interfaces. In this work, we focus on the two-domain approach, which decomposes the problem into two disjoint subdomains. The free-flow region is described by the Navier-Stokes equations while Darcy's or Forchheimer's law is used in the porous-medium subdomain. Appropriate coupling conditions are formulated at the common interface, which enforce the conservation of mass, momentum and energy. In this work, we present a novel mass and momentum conservative control-volume finite-element (CVFE) scheme for the discretization of the free-flow subdomain. Furthermore, a new approach to couple this CVFE scheme, which is used in the free-flow subdomain, with a vertex-centered finite-volume method (Box method), used for solving Darcy flow in the porous medium, is presented. This work is therefore an extension of the work presented in [Schneider et al., 2021, arXiv:2112.11089], where a staggered grid approach has been used to discretize the free-flow region. The advantages of the novel control-volume finite-element scheme and the new coupling approach are discussed in detail based on various test cases, ranging from convergence tests to real applications.

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MS21

Broadband Data-Driven and Physics-Based Earthquake and Shaking Simulations

Data-driven and physics-based inferences on earthquake source and shaking dynamics are challenged by the computational expense of the forward problem. Here we show pathways to overcome this challenge as (1) designing broadband earthquake dynamic rupture scenarios from low-resolution models (Taufiqurrahman et al., GRL 2022); (2) a joint coseismic and postseismic Bayesian dynamic source inversion (Premus et al., Sci. Adv., 2022) using the Parallel Tempering Monte Carlo algorithm to the well-studied 2004 Parkfield earthquake where observations can constrain the fault slip kinematics from the surface to the base of the crust and (3) instantaneous physics-based ground motion maps using reduced order modeling.

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MS21

Neural Operator-Based Hessian-Preconditioned MCMC Methods for Bayesian Inverse Problems

Many methods for Bayesian inference, such as MCMC and HMC samplers, can be greatly accelerated by preconditioning with the inverse Hessian (of the negative log posterior), constructed either locally or globally. The Hessian is very costly to form (each column formally requires a linearized forward PDE solve, and even low rank approximation methods still require a number of PDE solves that scale with the information content of the data. This makes preconditioning by local Hessians—ideal because they capture local correlation structure—intractable for large-scale problems. We address this challenge by constructing parametric surrogates of the parameter-to-observable map in the form of neural operators that are trained not just on function values, but also on the Jacobian of the map. This requires careful exploitation of the low rank structure of the Jacobian. Derivatives (of the outputs w.r.t. the inputs) of the neural operator are then used to build parameterized Gauss-Newton Hessian approximations, which in turn are used to precondition MCMC samplers. Numerical experiments on challenging Bayesian inverse problems demonstrate the large gains in sampling efficiency resulting from this approach.

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MS21

SymAE: An Autoencoder with Embedded Physical Symmetries for Passive Time-Lapse Monitoring

Many physical systems encountered in imaging applications are described by hidden states and are indirectly observed through repeated measurements corrupted by unmodeled nuisance parameters. We propose a network-based representation which learns to disentangle the coherent information (relative to the state) from the incoherent nuisance information (relative to the sensing). Instead of physical models, the representation uses symmetry and stochastic regularization to inform an autoencoder architecture called SymAE. It enables redatuming, i.e., creating virtual data instances where the nuisances are uniformized across measurements.

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MS22

Poroelasticity from DEM at Pore-Scale to Nonlinear Biot at Darcy Scale

Computational models of poroelasticity including the linear Biot model are well known. However, information on how the material properties such as permeability depend on the state of deformation is not easily available from empirical measurements. In the talk we present our steps towards determining the dependence of k on the deformation from computational experiments at the pore-scale. We start with quasi static assemblies of particles constructed with DEM (Discrete Element Method), which we post-process and follow up with CFD (Stokes flow) simulations. These are next upscaled to deliver the permeability and porosity dependence on deformation. These are used at Darcy scale.

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MS22

Parameter Identification in Hydro-Poromechanics by Physics-Informed Neural Networks

Physics-Informed Neural Networks (PINNs) are an innovative machine learning technique combining a standard data-driven training with the physics of the monitored process. In addition to data, these neural networks consider information from the governing equations by including the residual as a constraint in the training. A PINN-based approach is presented to reproduce coupled flow and deformation processes in geological porous media. In particular, we aim to use PINN for inverse modelling purposes and identify hydraulic and geomechanical parameters characterizing the material properties in the governing hydro-poromechanical equations. By leveraging previous work results, the coupled PDEs with unknown material coefficients are encoded to the PINN, so as to guess the values by relying on recorded measurements and simultaneously approximate the solution. The method is tested on classical benchmarks and the effect of different assumptions - e.g. quantity, location, noisiness of available data - on the identification accuracy is analyzed. Since PINN enables the discovery of a possible parameter space-dependence, an investigation of the technique in a heterogeneous setting is proposed too. The goal is to validate the approach capability to deal with problems in hydro-poromechanics, thus laying the foundation of the method in real-world geophysical applications.

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MS22

Governing Deterministic Equations at the Macroscale for Flow, Diffusion, and Deformation of Saturated Soils with and Without Swelling Clay

There are several ways to derive governing macroscopic equations for multiphysics porous media problems, among them homogenization and volume averaging (upscaling balance and constitutive equations) and hybrid mixture theory (upscaling balance equations and using the second law of thermodynamics to formulate the form of macroscale constitutive equations). Here we summarize the results of using the Hybrid Mixture Theory framework and present the macroscale equations for flow, deformation, and wave propagation. We also present the results of extending the results to swelling porous media such as soils containing shale and montmorillonite.

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MS22

Semilinear Degenerate Biot-Signorini System

Nonlinear extensions of the quasi-static Biot model of consolidation are studied with emphasis on boundary conditions, attainment of initial values, and parabolic regularizing effects. The local fluid content is monotone and possibly degenerate with respect to pressure, and the stress in the fully-saturated porous medium is strictly monotone in strain. The dependence of fluid flow on the pressure gradient and the two-way coupling via fluid pressure gradient and solid strain rate are linear. In addition to boundary conditions of classical Dirichlet, Neumann or Robin type for pressure and displacement on respective parts of the boundary, the medium may have a singular or degenerate semipermeable interface with the exterior fluid at a known pressure, and the dependence of traction on boundary displacement is monotone. This includes unilateral constraints on boundary displacement of Signorini type given by a variational inequality. The initial-boundary-value problem for this general system is formulated as a Cauchy problem in Hilbert space for a semilinear implicit evolution equation that is nonlinear in the time derivative, and it is shown to be well-posed with regularity of the solution dependent on the data. When the stress is the derivative of a convex strain energy function, the evolution equation is a gradient flow with corresponding parabolic regularizing effects on the solution.

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MS23

Preconditioned Newtons Method for Richards Equation

Richards equation is one of the most popular hydrogeological models that can be used to predict the movement of subsurface waters under both saturated and unsaturated conditions. However, despite its importance for hydrogeological applications, this equation has a bad reputation for being difficult to solve numerically. Indeed, depending on the flow parameters, the resolution of the algebraic systems arising from the discretization may become a very challenging task, as the linearization schemes such as Picard or Newtons methods may break down or exhibit unacceptably slow convergence. Nonlinear preconditioning is a powerful tool that may help to overcome the limitations of traditional nonlinear solvers both in terms of robustness and efficiency. As it is in the linear case the idea consists of replacing the original algebraic system with an equivalent one that can be solved by an iterative method more efficiently. In this presentation, I will review some traditional techniques involving the primary variables substitution and switching as well as some recent ones based on the nonlinear versions of Jacobi and Schwarz methods. The latter family of methods appears to be a very attractive option as it allows for the global convergence analysis in the framework of the Monotone Newton Theorem.

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MS23

Robust Newton Solvers for Richards Equation in Physical Formulation

We are interested in the numerical resolution of Richards equation modeling unsaturated flows in porous media, which writes

$$\phi\partial_t s - \nabla \cdot \left(\frac{k_r(s)}{\mu}\mathbb{K}(\nabla p - \rho g)\right) = 0.$$

The saturation s and the pressure p are linked by the monotone relation $s = \mathcal{S}(p)$ for some continuous non-decreasing function $\mathcal{S}$ which tends to 0 as p goes to $-\infty$ and which is constant equal to 1 as $p \geq 0$. It is well known that naive solvers based on Newton's method using p as a main variable suffer from a lack of robustness in the case of dry media because of the degeneracy $k_r(0) = 0$, whereas modified Picard solvers also face serious difficulties to converge in this regim. On the other hand, the choice of s as a primary variable does not allow to describe saturated zones since $p \geq 0$ is not a function of s. In this work, we propose an approach based on the parametrization of the monotone relation $s = \mathcal{S}(p)$ which, when combined with finite volumes, allows to solve efficiently Richard's both in the dry and saturated regims with Newton's method. This presentation is based on collaborations with Sabrina Bassetto, Konstantin Brenner, Guillaume Enchry and Quang-Huy Tran.

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MS23

Adaptive Regularization, Discretization, and Linearization for Nonsmooth Problems Based on Primal-Dual Gap Estimators

We consider nonsmooth partial differential equations associated to the minimization of an energy functional. We adaptively regularize the nonsmooth nonlinearity so as to be able to apply the usual Newton linearization, which is not always possible otherwise. Then the finite element method is applied. We focus on the choice of the regularization parameter and adjust it on the basis of an posteriori error estimate for the difference of energies of the exact and approximate solutions. Importantly, our estimates distinguish the different error components, namely those of regularization, linearization and discretization. This leads to an algorithm that steers the overall procedure by adaptive stopping criteria with parameters for the regularization, linearization, and discretization levels. We prove guaranteed upper bounds for the energy difference and discuss the robustness of the estimates with respect to the magnitude of the nonlinearity when the stopping criteria are satisfied. Numerical results illustrate the theoretical developments.

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MS23

A Robust and Reliable L-Scheme/Newton Switching Algorithm for Richards Equation

Richards equation describes subsurface flow of both saturated and unsaturated conditions. It is a highly nonlinear, and possibly degenerate equation which imposes significant challenges in obtaining numerical solutions. Typical linearization schemes such as Picard or Newtons method may fail to converge and more robust methods like the L-scheme might exhibit slow convergence. In this work, we propose an adaptive, robust and reliable a-posteriori based switching algorithm between the L-scheme and Newton's method. Hence, we utilize the quadratic convergence of Newtons method and the robustness of the L-scheme. The performance of the algorithm is compared to the L-scheme and Newtons method through realistic examples. For these examples, the number of iterations and the computational times are presented.

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MS24

A Fully-Coupled Highly-Parallelized Geomechanical Simulator

High-pressure fluid injections cause modification of the subsurface effective stress state and transient pore pressure changes over large distances, which could induce seismicity. It has been observed in a number of industrial applications – from hydrocarbon extraction, drilling waste-water disposal to the hydraulic stimulation of deep geothermal systems leading to the termination of the project in some cases. These activities change the stress state of a rock formation at kilometres depth and perturb the balance on existing faults, possibly causing them to slip. It is crucial to evaluate possible fault reactivation already at the design stage. We propose a numerical model capable of predicting behaviour of rock formation subject to fluid injection or extraction. A poroelastic formulation is used to describe the behaviour of the porous rock. The finite-element method is used to solve both the mechanical deformations of the rock and the fluid flow in the matrix. High efficiency and scalability of the simulator is achieved by using MPI routines, which makes it capable of large-scale simulations. We present several benchmarking tests to demonstrate efficiency of the model.

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MS24

Energy Stable Discretizations of Thermo-Poro-Elastic Models in Fractured Porous Media

We consider in this work a Thermo-Hydro-Mechanical (THM) model in fractured porous media for which fractures are represented as co-dimension one interfaces. The model couples the mixed-dimensional non-isothermal single phase flow, the matrix thermo-poro-elastic model and the mechanical behavior of the fractures based on Coulomb frictional contact. This type of models plays in important role in several applications such as e.g. the hydraulic stimulation of deep geothermal systems, or the risk assessment of induced sismicity in CO2 storages. Compared with the isothermal case, the thermal coupling induces additional difficulties related in particular to the nonlinear convection terms. Starting from the pioneer work of Coussy [2004], we introduce a thermodynamically consistent discretization of the THM coupled model which naturally leads to a discrete energy estimate. Our approach covers various types of finite volume discretizations of the non-isothermal flow which can be either cell-centered, nodal or hybrid. It accounts for a wide range of thermodynamical single phase fluid model and of thermo-poro-elastic parameters, as well as for any Peclet number in the energy transport. The efficiency of our approach will be assessed on several 2D benchmark test cases.

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MS24

Modeling Thermo-Poroelastic Response of Fractured Media in Energy Transition Applications

Energy transition applications such as geothermal energy production and CO_2 sequestration change reservoir temperature due to colder fluid injection (as in geothermal) or adjustment of the energy in situ (like Joule-Thomson cooling in CCS). Changes in the reservoir pressure and temperature impact the stress field. In naturally fractured or faulted reservoirs, stress changes introduce risks of fault reactivation and induced seismicity. Moreover, stress changes dynamically adjust apertures in fracture network, which can significantly impact reservoir performance. In this study, the capabilities of the Delft Advanced Research Terra Simulator (DARTS) framework have been extended to account for the thermo-poroelastic response relevant to geothermal applications. A similar approach can be directly extended for CO_2 sequestration applications. In the proposed modeling approach, the flow and heat transfer through natural fractures are represented by the Discrete Fracture Model. A low-fidelity model is used for geomechanics where stresses are calculated from pressure and temperature changes. Fracture apertures are updated according to stresses and the fault slippage is calculated using Mohr-Coulomb friction criteria. The developed model has been applied to heterogeneous geothermal fields to evaluate how energy production and thermal front can affect the geomechanical state of the field and trigger induced seismicity.

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MS25

Plant Roots Inpainting

Plant roots are the main actor in the transfer of water from the soil to the atmosphere. The precise identification of their structure is crucial to simulate coupled multiphysics problems that involve the soil-plant-atmosphere continuum. Currently, the identification of root networks in soil via noninvasive imaging techniques is an extremely challenging problem. Due to noise and/or resolution limits, we often only have access to corrupted reconstruction of the roots structure, with disconnection that are hard to detect and remove (a process called inpainting). Variational image processing methods can reconstruct root networks as a result of a minimization problem that involves a discrepancy measure and penalization terms. However, standard penalization functionals used in image processing are not suitable for the plant roots reconstruction problem. They are often norms that capture only local information and do not express any physical concepts. They ignore our knowledge that we are dealing with a transport network. In this talk we will show how the Optimal Transport theory can provide a new mathematical tool to encode into equations this key information. We will present some preliminary experiments where these ideas are tested.

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MS25

Pore Scale Modelling of Evolving Soil Structures

Although advanced imaging techniques now allow snapshots even down to the nanoscale, the evolution of particle distributions, different liquid phases and dynamic microbial communities still cannot be assessed fully in experiments. Consequently mechanistic models operating at the pore scale facilitate the study and understanding of such intimately linked phenomena. We present a versatile hybrid discrete continuum modeling approach combining cellular automata and partial differential equations which integrates the complex coupling of biological, chemical, and physical processes (e.g. Rupp et al. 2018, Discrete-continuum multiphase model for structure formation in soils including electrostatic effects, Front. Env. Sci. 6, 96). A focus lies on a dynamically evolving solid phase, capturing the self-organization by aggregation of soil particles, growth of biofilms, roots, or the distribution of particulate organic matter in the system. Finally mathematical homogenization techniques are used to show a way to incorporate information as the diffusivity from the pore scale (based on CT scans) to macroscale models. Applications include the interplay of organic matter turnover and aggregate formation relevant for CO2 storage (Zech et al. 2022, Explicit spatial modeling at the pore scale unravels the interplay of soil organic carbon storage and structure dynamics, Glob. Ch. Biol. 28, 15), or the influence of root exudates on structure development in the rhizosphere.

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MS26

Surrogate Models for Fractured Porous Media

We create surrogate models of flow in fractured porous media capable of accurately solving different scenarios in a short computational time. We compare two different techniques: one is based on a linear map from the original to the reduced space, and the other one on a non-linear map. For the linear approximation, we assess the proper orthogonal decomposition (POD), implemented both in a monolithic approach, that is computing a unique set of basis for the representation of the reduced space, and a block approach, which means computing as many subsets of basis as the number of physical variables. Then, we assess a non-linear technique based on the sole use of Neural Networks (NNs), exploiting their ability to efficiently approximate high dimensional and nonlinear maps. We consider different NNs architectures that connect multiple NNs pursuing different approximation tasks. We apply these techniques to different problems with variable physical properties and geometry. In order to change the geometry, we pay particular attention to the treatment of the grid deformation of a non-conforming mesh. Generally speaking, it is possible to reach satisfying accuracy for both methods. The comparison shows that the POD technique takes a shorter time during the offline stage w.r.t. the NN approach, whereas the latter generates a model whose online stage is orders of magnitude faster than the former.

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MS26

Pore-Scale Transport Simulations on Microct Images Enabled By Super Resolution Generative Adversarial Networks

Achieving image super resolution would lead to significant breakthroughs in understanding of dynamic properties of rocks by increasing image resolution and throughput. Improved resolution improves accuracy of prediction of rock properties. Toward this goal, we show super resolution of CT images using deep learning. Generative Adversarial Networks (GANs) and diffusion models were implemented to remove noise while preserving image content. GAN's employ a predictor-corrector architecture while the diffusion model reduces noise. The data set is from a sandstone that is being evaluated for its CO2 storage potential. Evaluation of flow characteristics is needed for engineering decisions. The field samples were imaged with a clinical Computed Tomography (CT) scanner (100s micron) as well a microCT scanner (sub 10 micron). Dynamics of single-phase flow as well as simultaneous CO2 and brine flow were measured at low resolution. Results illustrate the potential for deep learning to improve image resolution of CT images by at least a factor of 4. Image improvement is measured by computing various Minkowski functionals including surface area and Euler characteristic. Images then resolve rough rock grains, microfractures, and other fine-scale features.

Super resolved images are then used as input for computation of single and two-phase flow (pressure drop versus flow rate, CO2 and brine volume fraction) that show good predictability of laboratory measurements.

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MS26

Data-Driven Modelling with Coarse-Grid Network Models

Any standard discretized reservoir model can be seen as a data-driven network model, in which pore volumes and relative permeabilities are node parameters and transmissibilities edge parameters. If we, unlike in history matching, disregard prior geological knowledge and the physical meaning of the parameters, we are left with a network with many freely adjustable parameters. We show that networks with surprisingly low granularity (tens to hundreds of nodes) can be tuned to match complex responses accurately. The models are trained using Levenberg-Marquardt to minimize misfit. This requires the full parameter-to-output sensitivity matrix but is viable since our network models are so small that we can efficiently compute this matrix in a single adjoint sweep. Unlike interwell networks that represent the reservoir as flow paths connecting injectors and producers, the data-driven version of our approach derives the network from a minimal rectilinear mesh covering the map outline and base/top surface of the reservoir. This gives more flexible networks. We also show how network granularity can be iteratively enhanced to obtain a given mismatch tolerance. We discuss the ability to predict responses outside the training data, both by analysis and by considering numerical observations. Finally, we present numerical examples in which models are calibrated to output from detailed simulation models. We consider both standard black-oil models and models for geothermal heat storage.

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MS26

Data-Driven Homogenization for Coupled Porous-Medium and Free-Flow Systems

Coupled porous-medium and free-flow systems appear in a wide range of environmental settings and industrial applications. Generalized coupling conditions, which are valid for arbitrary flow directions, have been recently developed using homogenization and boundary layer theory. These conditions contain several effective parameters which must be computed for each porous structure. Accurate estimation of these effective properties is important for physically consistent modelling and accurate numerical simulation of flow and transport processes in coupled flow systems. This computation can be significantly accelerated using neural networks, especially for complex non-periodic porous structures. In this talk, we present the study on the neural networks for an accurate estimation of permeability and boundary layer constants appearing in the generalised interface conditions. A fully trained convolutional neural network requires a fraction of the computation time required by mathematical homogenization in order to accurately predict effective model parameters.

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MS27

Bayesian Inversion for Earthquake Recurrence Using Chlorine-36 Measurements

An emerging approach for determining earthquake slip histories on faults is to analyze the surface exposure of rocks, estimated by the abundance of the isotope chlorine-36 (36Cl). In this presentation, we present a Markov-chain Monte Carlo (MCMC) algorithm for the inference of timings of past ground displacements from 36Cl measurements in limestone rocks along the fault plane. Such results are valuable for studying earthquake recurrence and for seismic hazard assessments. To solve this Bayesian inverse problem, we utilize computer simulations of 36Cl accumulation for a set of fault-scarp rock samples from the fault scarp, progressively exhumed during earthquake events, and 36Cl measurement data. We compare the inferred earthquake intensity over time with a historical record for validation. The Fiamignano and Frattura faults in the Italian Apennines are the case studies considered. Our results show that in addition to the variability in inter-event times around a constant slip rate, these faults show heightened activity and quiescence over periods lasting a few millennia relative to the longer-term deformation rate.

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MS27

Bayesian Experimental Design for the Optimal Network of Sensors in Seismic Moment Tensor In-

version

Efficiency in analyzing the uncertainty of the earthquake mechanism is typically difficult due to the lack of degrees of freedom on the data collection process. We propose a methodology to advance the inversion of the seismic moment tensor by optimizing the locations of a limited number of sensors. The Shannon expected information gain is used as the objective function to search the optimal network of sensors. A closed form of it results due to the linear structure of the seismic displacements obtained with the Greens function formulation, together with the Gaussian characterization of the prior knowledge, and the Gaussian structure of the measurement errors. To alleviate the computational load inherent in the resulting combinatorial optimization problem, a greedy algorithm is deployed to sequentially select the sensor locations that form the best network for learning the moment tensor. Numerical results are presented to display the optimal network of sensors and how the uncertainty in the inferred seismic moment tensor contracts. We also show the robustness of the method for efficiently estimating the moment tensor for full three-dimensional velocity-models or when the earthquake-source location is unknown by examining a consensus approach over a set of representations of the velocity field or over a set of guessed of the earthquake-source locations.

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MS27

Bayesian Traveltime Tomography Using Surrogate Models

This talk is about the issue of the computational load encountered in seismic imaging by Bayesian traveltime inversion. In Bayesian inference, the exploration of the posterior distribution of the velocity model parameters requires extensive sampling. The computational cost of this sampling step can be prohibitive when the first arrival traveltime prediction involves the resolution of an expensive number of forward models based on the eikonal equation. We propose to rely on polynomial chaos surrogates of the traveltimes between sources and receivers to alleviate the computational burden of solving the eikonal equation during the sampling stage. The numerical tests for canonical problems (simple layered media, microseismic and seismic refraction configurations) illustrate that a moderate number of evaluations of the eikonal solver suffices to build traveltime surrogates with an error less than the typical observation noise. When constructed, the surrogates of the traveltimes enable the extensive sampling of the posterior distribution with Markov Chain Monte Carlo methods. Our experiments show that the posterior uncertainty in the velocity model parameters depends on the observations available and the structural dependencies between the parameters and the traveltimes. The seismic refraction configuration also highlights the potential of relying on advanced surrogate construction methods, suited to the posterior distribution, through an iterative adaptation.

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MS28

Modelling Complex Physics and Multi-Phase Flow Within a Black-Oil Reservoir Simulator

Black-oil reservoir simulators are potentially faster than the compositional simulators, and much simpler to setup cases and calculations. Faster and simplified models are needed for use in workflows of field developments studies (uncertainty quantification, model calibration and operational optimization, risk assessment, etc.). We have been working on extending the black-oil formulation to model complex physics in multi-phase flow, as e.g., modeling of salt precipitation and water evaporation, Joule-Thomson thermal effects, and CO_2/H_2 storage. We propose a translation of compositional models into a black-oil model description. Special attention needs to be given on translating PVT properties and retaining relevant physical aspects. First evaluations of the performance and accuracy of an open-source black-oil simulator (OPM-flow) modified with our proposed approach shows very promising results comparing the simulation results obtained with OPM-flow against those of an industry-standard commercial compositional simulator.

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MS28

The Unified Isenthalpic Flash Procedure for Simulation of High-Enthalpy Geothermal Systems

In simulation of high-enthalpy geothermal systems, the theory of compositional flow in porous media provides a powerful modeling framework to gain insight into the subsurface processes. In this setting, two classic problems - heat and mass transfer and the thermodynamic equilibrium problem - pose one coupled problem. The system is characterized by the presence of various chemical species, each of which may be present in vapor and liquid phase. Recent advances in modelling and analysis of the unified formulation for multiphase mixtures enable us to treat the phase stability (appearance/ disappearance) and phase split calculation in a closed manner, with the potential to reduce the complexity of numerical schemes and increase their efficiency. In this work, the unified approach is utilized and extended to formulate an isenthalpic flash procedure, coupled with the transport of mass and energy. The closed formulation of the unified approach is utilized to construct a numerical scheme for the coupled problem based on a non-linear Schur elimination. The proposed algorithm is tested on the simulation of a high-enthalpy geothermal system using a NaCl-H2O brine model. Essential modelling and simulation steps are provided, and the advantage of the isenthalpic formulation in high-enthalpy systems is demonstrated.

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MS28

Using Robust and Efficient Multiphase Thermodynamics for Modelling of Energy Transition Applications

Phase behaviour plays an important role in subsurface flow and transport related to energy and environmental applications, including CO2 sequestration, geothermal energy and hydrocarbon-related activities. In case of full-physics compositional reservoir simulation, calculation of complex thermodynamics and accurate phase behaviour is often computationally intensive and a determining factor in simulation performance. Moreover, a single failure in thermodynamic calculations will cause error propagation, leading to false solutions or failures of the simulation. In this work, we present advanced methods for thermodynamic modelling, incorporated into the Delft Advanced Research Terra Simulator (DARTS) platform, an efficient compositional framework for full-physics reservoir simulation. Based on the advanced second-order methods for phase behavior evaluation, strategies for thermodynamic modelling of a range of problems, involving brine, various non-aqueous fluid and solid phases will be presented in this study. In addition to the capabilities related to multiphase equilibrium, the DARTS framework includes a flexible implementation of kinetic reaction mechanisms, extending the abilities to describe a wide range of complex thermal-compositional-reactive phenomena. The application of the thermodynamic package will be demonstrated in a set of simulation scenarios relevant to energy transition applications.

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MS29

Value of Local Data and Predictability in Numerical Simulation of Geologic Co2 Storage

The accuracy of physics-based models of geologic carbon sequestration is rarely quantified with respect to a clearly defined ground truth. To close this gap, we present a set of CO_2 injection experiments in meter-scale, quasi-2D tanks with transparent sides and combine them with numerical simulations of the experiments. We evaluate (1) the value of prior knowledge of the system, via local measurements of the quartz sands in the tank, to obtain an accurate simulation; and (2) the predictive ability of the matched numerical models, when applied to different injection scenarios and stratigraphic sections. To achieve this, we match three different models, each with access to an increasing level of local data, to CO_2 injection experiments in tank 1 ($89.7 \times 47 \times 1.05$cm). Matching is based on a quantitative comparison of CO_2 migration, as determined from timelapse images. Next, we use the three matched models to simulate a different injection in the same tank, and, finally, a different injection scenario in tank 2 ($2.86 \times 1.33 \times 0.019$m), which contains a different stratigraphic section. Results show that all models can qualitatively match CO_2 plume migration and convective mixing to the experimental truth. However, using local data reduces the time required to obtain a satisfactory match, and improves the quantitative match with the experiment as well as the predictive capability of our models.

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MS29

An Open-Source Image-Based History Matching

Framework for the FluidFlower Data Set

There are relatively few large-scale projects when it comes to CO_2 storage, which means that it is necessary to increase knowledge about CO_2 flow, as well as validate and calibrate the models and workflows we use. This is where FluidFlower comes in as a tool where, unlike a real reservoir, we have control over model parameters and the opportunity to visually observe the CO_2 dynamics in the reservoir. Access to high-resolution images of CO_2 flooding provides a unique opportunity to validate the simulation models as well as explore parameter sensitivity and workflows for history matching. In this talk, we present results of performing history matching studies on the benchmark FluidFlower data set using OPM Flow for the numerical simulations and ERT as the history matching toolbox. First, we introduce the open workflow 'pyff, a Python package to set up the studies via a configuration file. This gives researchers and lecturers a simple and transparent way to compare experiments and modeling. Second, we examine different setups for history matching of tracer and CO_2 data. In particular we compare using pixel based data at some given time-intervals with using averaged quantities in some given boxes. The pixel based data is motivated from seismic while the average box values resembles well type data.

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MS29

Simplified Numeric Simulation Approach for CO2,g-Brine Flow and Trapping at Near-Surface Conditions

The Fluid Flower study (Nordbotten et al., 2020). To simulate $CO_{2,g} - brine$ flow in this tank, subject to viscous, gravitational and capillary forces as well as the dissolution ($CO_{2,aq}$), we constructed a simple pseudo black-oil model, discretizing the governing equations on a collocated finite element finite volume (FE-FV) mesh using operator splitting and a sequential solution approach. Simple PVT correlations were used for gas density, viscosity, and solubility as based on experimental studies and equations of state from the literature. These solubility calculations assume instantaneous chemical equilibrium. The simulator captures the expected physical phenomena such as capillary filtration, gravitational segregation, and dissolution fingering. The error in the total mass, due to ignoring solubility variations with pressure remains acceptable as long as the pressure variation in the tank is small.

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MS29

Simulation of CO2 Storage Using a Parameterization Method for Essential Trapping Physics: FluidFlower Benchmark Study

An efficient compositional framework is developed for simulation of CO2 storage in saline aquifers during a full-cycle injection, migration and post-migration processes. Essential trapping mechanisms, including structural, dissolution, and residual trapping, which operate at different time scales are accurately captured in the presented unified framework. In particular, a parameterization method is proposed to efficiently describe the relevant physical processes. The proposed framework is validated by comparing the dynamics of gravity-induced convective transport with that reported in the literature. Results show good agreement for both the characteristics of descending fingers and the associated dissolution rate. The developed simulator is then applied to study the FluidFlower benchmark model. An experimental setup with heterogeneous geological layers is discretized into a two-dimensional computational domain where numerical simulation is performed. Impacts of hysteresis and the diffusion of CO2 in liquid phase on the migration and trapping of CO2 plume are investigated. Inclusion of the hysteresis effect does not affect plume migration in this benchmark model, whereas diffusion plays an important role in promoting convective mixing. This work casts a promising approach to predict the migration of the CO2 plume, and to assess the amount of trapping from different mechanisms for long-term CO2 storage.

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MS30

A 3D Coupled VEM-MFD Formulation for Multiphase Flow and Poromechanics

The simulation of underground deformations induced by flow in real scenarios can, in many cases, be limited or slowed down by meshing issues, especially when the numerical discretization methods are limited to polyhedra of standard shape, such as tetrahedra or hexahedra. New generation numerical methods such as Mimetic Finite Differences (MFD) [K. Lipnikov et al., Mimetic finite difference method, 2014] and Virtual Element Methods (VEM) [L. Beiro da Veiga et al., A Virtual Element Method for elastic and inelastic problems on polytope meshes, 2015], can help circumventing such issues, since they allow for more general star-shaped polyhedra and treat aligned edges and aligned faces naturally. We describe a fully coupled 3D scheme of multiphase flow and poromechanics, where MFD are used to discretize the flow equations and VEM are used for mechanics (the 2D version of the method was proposed in [A. Borio et al., Hybrid mimetic finite-difference and virtual element formulation for coupled poromechanics, 2021]). The method has the interesting feature of allowing the use of polyhedral meshes. We present some standard tests validating the method and some results on realistic domains obtained by an optimized implementation of the scheme carried out within a massively parallel open source multiphysics simulator (https://www.geosx.org).

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MS30

An Oscillation-Free Numerical Scheme for the Biot's Model

In this talk, we present a new stabilization method to remove the non-physical oscillations in the pressure approximation of Biot's model for low permeabilities and/or small time steps. We consider different finite element discretizations and illustrate how such a stabilized scheme provides solutions free of spurious oscillations. The new scheme allows us to directly iterate the fluid and mechanics problems similarly to the well-known iterative coupling methods, as the fixed-stress split method for example. Numerical results are presented to illustrate the good behavior of both the stabilization and iterative solver with respect to the physical and discretization parameters of the model.

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MS30

Direct and Inverse Problems for Elastic Dislocations in Geophysics

I will discuss both direct and inverse problems for certain models of flow and fractures in the Earth's crust. the inverse problem consists in determining the geometry and location of the fault or fractures from boundary measurements under some conditions. The slip can also be determined. I will briefly discuss a recovery algorithm based on a shape derivative if time permits.

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MS31

Diffuse Interface Method for the Interaction Between Flow and Porous Medium

We will begin by introducing a Stokes-Darcy coupled problem describing the interaction between a free flowing a porous medium. To solve this problem numerically, we use a diffuse interface approach, where the weak form of the coupled problem is written on an extended domain which contains both Stokes and Darcy regions. This is achieved using a phase-field function which equals one in the Stokes region and zero in the Darcy region, and smoothly transitions between these two values on a diffuse region of width $\mathcal{O}(\epsilon)$ around the Stokes-Darcy interface. We will show the proof of the convergence of the diffuse interface formulation to the standard, sharp interface formulation, and the obtained rates of convergence. We will then talk about the applications of this method and extensions to Stokes-Biot coupled problem.

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MS31

Time-Splitting Methods Based on Robin Coupling Conditions

We apply a loosely coupled splitting method based on Robin-type coupling conditions to classical coupled problems such as the fluid-structure interaction problem. In the case of a static interface, this coupled splitting method has been proven to be unconditionally stable with quasi-optimal error estimates in time, although this behavior can be delayed significantly when the values of the physical parameters are large. Critically, however, the value of the parameters does not impact the unconditional stability, so the splitting method does not suffer from the added-mass instability common to other loosely coupled methods. We discuss these results in time-semi-discrete and fully discrete frameworks. We then discuss the extension of these results to the case of a moving interface and the necessary adjustments for optimal and higher-order accuracy in time.

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MS31

Hyperbolic System and Explicit Scheme for Tightly Coupled Buoyant Two-Phase Flow and Transport in Porous Media

Buoyant incompressible multiphase flow and transport in porous media typically is simulated by coupling an elliptic flow equation with a hyperbolic transport description. The tight coupling between flow and transport either requires a fully implicit solution algorithm or very small time steps, if solved sequentially. In any case, however, a large linear system has to be solved each time step. Here, a new solution approach is presented, which relies on solving a coupled hyperbolic system of conservation laws with an explicit finite volume method. Consequently, only local operations have to be performed, which is a great advantage in case of massive parallel simulations and if GPUs are employed. The devised method is based on the isothermal Euler equations with momentum source terms accounting for resistance due to the porous medium and buoyancy. In this system the pressure is proportional to the density and in case of very small Mach numbers and relative density variation, the computed velocity field is divergence free and converges towards the total volumetric flow in the porous domain. To account for saturation transport, the system was augmented by an additional hyperbolic equation. In order to obtain the numerical fluxes, a characteristic based approximative Riemann solver was developed and 2nd order accuracy in space and time is achieved by piecewise linear reconstruction.

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MS31

A Partitioned Method for the Solution of Fluid-Structure Interaction and ROM Implementation

Partitioned methods for the solution of fluid-structure interaction (FSI) problems are often the preferred approach as they allow the reuse of existing codes for each subdomain that take into account its unique mathematical and physical properties. We present a partitioned method for FSI problems based on a monolithic formulation of the problem, which employs a Schur complement equation for a Lagrange multiplier. This algorithm eradicates the need for iterations between the fluid and structure subdomains and instead allows them to be decoupled and solved separately at each time step. The Lagrange multiplier, representing an approximation of the interface flux, serves as a Neumann boundary condition for each sub-problem, allowing for the fluid and structure to be solved independently at each time step. To reduce computational costs, we consider implementing a reduced order model (ROM) for one or both subdomains. The Schur complement method developed for the original FSI scheme can be utilized to couple a reduced order model with either a full order model or a reduced order model on the other subdomain. We show numerical results demonstrating the methods capability to capture each type of coupling.

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MS32

Spectral Decomposition-Based Deep Learning Using Attention U-Net for Improved Automated Seismic Segmentation

Facies mapping from 3D seismic is of significant value to various interpretation and characterisation tasks. Traditional manual facies mapping is based on the analysis of sedimentary environments and stratigraphic sequences. Typically this task is time and labour consuming, which is further increased with the ever-growing size of seismic data sets. In this study, we investigate the application of machine learning techniques, particularly state-of-the-art deep convolutional neural networks (CNNs), as a framework to perform automated seismic facies pixel-wise segmentation. The workflow consists of a CNN based U-Net architecture with three additional add-ons to boost the performance of the standard U-Net: (1) using residual building blocks in the encoder (2) using transformer like attention gates after each residual block, and (3) using frequency spectrum, in addition to seismic amplitude, as input to the network. We show that this implementation achieves higher accuracy outperforming state-of-the-art U-Net architecture. The performance of the proposed method is validated using the F3 Netherlands data set and the Penobscot data set acquired offshore Canada. Experimentation involves training and hyper-parameter tuning on a set of samples, followed by quantitative evaluation of the trained network. The proposed workflow in this work demonstrates significantly reduced artifacts, improved edge detection, and improved lateral consistency.

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MS32

Digital Twins for the Subsurface, How Far Can We Go?

It is now firmly grounded that digitalisation of the subsurface is an essential tool for exploration, field management and decision-making in many domain of geosciences, such as geothermal, CO2 storage, hydrogeology, mineral resources, geohazards. An over-arching principal is, to be able to confront the model with the data to mitigate the associated risk, and cost. Therefore, one has to be aware of the uncertainty encompassed within the process, including the technical inversion problem itself, which propagates uncertainty. In other industries, a strategy to reduce these uncertainties includes a digitization of the entire modeling process with an integration of prior knowledge, models, and systematic procedures for model updates. This process is often described as going from a digital model to a digital shadow and finally a digital twin, the latter being a perfect replica of the object under scrutiny. For the subsurface, one major challenge is our incapacity of measuring every points in space, whereas the configuration and state of fabricated objects can be known to a high accuracy, the same is arguably not the case for any realistic object of interest in the subsurface. Consequently, there is currently no consensus on the best practice to create digital twins and to assimilate data for model update. In this discussion, we propose to give an overview in data assimilation for the subsurface uncertainty-driven workflows and discuss other ways to look at the problem.

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MS32

Physical Residual Neural Networks for Reduced Order Modelling of Reactive Flow in Porous Media

Accurate prediction of solid mineral dissolution during reactive flow in porous media is vital for a wide range of subsurface applications (e.g., CO2 sequestration). Detailed numerical modelling of mineral dissolution at the pore-scale is generally expensive and that limits our ability to perform comprehensive uncertainty quantification studies to explore the various sources of uncertainties and its impact on the dissolution process. In this work, we develop an efficient deep learning emulators for geochemical reactions. We build on an earlier work on reduced order modelling (ROM) using Deep residual recurrent neural network to develop highly predictive ROM using limited training data. We utilize a U-net architecture to perform approximate explicit time stepping for the dynamical system. The input features for the deep learning model are the discrete components of the physical residual which are known to correlate well with the solution updates over the training samples as well as the unseen validation dataset. The developed algorithm is demonstrated on a dataset with different Peclet and Kinetic numbers. The pore-scale dissolution training and validation datasets are generated using detailed numerical simulations using the improved Volume-of-Solid method in GeoChemFoam and are available as an open access repository for a range of dissolution regimes.

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MS32

Effects of Iterative Learning on Machine Learning Performance for Geoenergy Problems

Machine learning is efficient in solving geoenergy problems, provided that the algorithm is designed as domain-specific to capture complex patterns in physical phenomena from big high-quality data with different sources. This study analyzes the effects of iterative learning on machine learning performance. Firstly, we synthesize high-resolution porosity data, whose resolution is identical to that of core data, from well-logging data for gas-hydrate-bearing sediments in the Republic of Korea. This downscaling is conducted through two learning stages. A neural network learns how to estimate high-resolution porosity by inputting well-logging and outputting empirical porosity. This model is re-trained by correcting porosity estimates to be in good agreement with core porosities. We also present another iterative-learning approach to determine the optimal well location during primary oil recovery using a multi-modal convolutional neural network (M-CNN). Particle swarm optimization provides the M-CNN with reservoir simulation results as learning data to correlate near-wellbore properties as inputs and oil production as output. The M-

CNN estimates oil productivity at every feasible location to find the most prolific location. Its prediction performance is improved by adding qualified locations in learning data and re-training the M-CNN. These applications reveal the significance of balancing accuracy and computational cost for the automated decision-making of geoenergy problems.

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MS33

Accelerating the Scientific Discovery Loop for Convection in an Idealized General Circulation Model

Climate models depend on dynamics across many spatial and temporal scales that cannot all be resolved. The physics at the smallest scales is represented by schemes to link what is unresolvable to variables resolved on the grid scale. A large source of uncertainty in climate predictions comes from the calibration of empirical parameters within these schemes, and uncertainty is generally not quantified. The uncertainties can be reduced and quantified with data that may be very limited in space and time, for example, data from a field campaign a limited-area high-resolution simulation. As the sensitivity of model outputs to parameterizations varies in space and time, this raises the question of where and when to acquire additional data so as to optimize the information gain from it. We construct an automated algorithm to finds optimal regions and time periods for data acquisition, to maximize the information the data provides about uncertain parameters. We use a Bayesian framework to characterize the uncertainty and apply the new Calibrate-Emulate-Sample (CES) methodology to accelerate its calculation. The combined algorithm is parallelizable and very efficient with respect to evaluations of the model. In proof-of-concept simulations with an idealized global atmosphere model, the algorithm successfully identifies informative regions and times, even in cases where physics-based intuition may lead to sub-optimal choices.

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MS33

Differentiable Programming for Hessian-Based Ocean Climate Observing System Design in the North Atlantic

Designing effective ocean observing networks benefits from quantitative strategies to mitigate heavy cost and logistical challenges of ocean observing. We leverage uncertainty quantification (UQ) via second-derivative, i.e., Hessian information within the ECCO (Estimating the Circulation and Climate of the Ocean) data assimilation framework to explore a quantitative approach for ocean climate observing systems. An observing system is considered optimal if it minimizes uncertainty in a set of investigator-defined design goals or quantities of interest (QoIs), such as oceanic transports or other key ocean indices. Hessian UQ unifies three design concepts: (1) An observing system reduces uncertainty in a QoI when it is sensitive to the same dynamical controls as the QoI, as quantified by the dynamic proxy potential. The dynamical controls are exposed by the Hessian eigenvector patterns of the model-data misfit function. (2) Orthogonality of the Hessian eigenvectors rigorously accounts for complementarity versus redundancy between distinct members of the observing system. (3) The Hessian eigenvalues determine the overall effectiveness of the observing system as characterized by the sensitivity-to-noise ratio of the observational assets, analogous to the statistical signal-to- noise ratio. We illustrate the framework in the design of an effective observing system in the subpolar North Atlantic that maximally informs the target QoIs.

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MS33

Bayesian Inference of Seafloor Deformation from Near-Source Pressure Observations with Application to Tsunami Forecasting

To improve tsunami preparedness, early-alert systems and real-time monitoring are essential. We propose a novel approach for predictive tsunami modeling within the Bayesian inversion framework. This effort focuses on informing the immediate response to an occurring tsunami event using near-field data observation. Our forward model is based on a coupled acoustic-gravity model (e.g., Lotto and Dunham, Comput Geosci (2015) 19:327–340). Similar to other tsunami models, our forward model relies on transient boundary data describing the location and magnitude of the seafloor deformation. In a real-time scenario, these parameter fields must be inferred from a variety of measurements, including observations from pressure gauges mounted on the seafloor. One particular difficulty of this inference problem lies in the accurate inversion from sparse pressure data recorded in the near-field where strong hydroacoustic waves propagate in the compressible ocean; these acoustic waves complicate the task of estimating the hydrostatic pressure changes related to the forming surface gravity wave. Furthermore, the forward model incurs a high computational complexity, since the pressure waves must be resolved in the 3D compressible ocean over a sufficiently long time span. Due to the infeasibility of rapidly solving the corresponding inverse problem for the fully discretized space-time operator, we explore options for using surrogate operators of the parameter-to-observable map.

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MS33

Bayesian Active Learning of Model Parameters in Rapid-Flow Geohazards

Model-based decision support tools for assessment and mitigation of risks due to rapid-flow type geohazards such as landslides, avalanches, and rock fall are gaining significant importance. Computational models used in such tools to assess impact area or the evolution of run-out, however, contain parameters that cannot be measured a priori, but need to be calibrated based on data from past events. We focus herein on a Bayesian parameter calibration approach to perform reliable predictions based on calibrated model parameters. Its application is challenging due to high computational costs resulting from a typically large number of required forward simulations. To overcome this computational bottleneck, we propose an efficient Bayesian parameter calibration strategy via integrating forward process models, Bayesian inference, Gaussian process emulation, and Active learning techniques. We summarize our conceptual approach in this presentation, and demonstrate results of an extensive synthetic case study. We find a significant reduction of overall compute time owing to the integration of Gaussian process emulation and Active learning. We furthermore apply our framework to test Bayesian inversion results for different sets of candidate data and close by presenting results from a real-world test cases, before concluding our findings.

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MS34

Challenges in the Estimation of the Wave-Affected Sea Ice Extent

As sea ice extent decreases in the Arctic with increasing temperatures, surface ocean waves have more time and space to develop and grow, exposing the Marginal Ice Zone (MIZ) to more frequent and energetic wave events. Waves can fragment the ice cover over tens of kilometres but the impact it has on the sea ice cover remains mostly unknown. The first obstacle to assessing this impact is the estimation of the extent over which waves can penetrate the ice cover. This estimation is extremely challenging as wave attenuation is due to competing mechanisms which depend on sea ice properties, and observations are scarce, limited in time and space. Numerical models can be used to complement observations and test hypotheses. Here, we introduce a new coupled framework involving the spectral wave model WAVEWATCH III and the sea ice model neXtSIM. To constrain the extent over which waves can impact the sea ice in our model, we evaluate the MIZ extent by comparing our model results to pan-Arctic wave-affected sea ice regions derived from ICESat-2 altimetry over the period December 2018 - May 2020. The model produces MIZ extent comparable to observations, especially in winter, but underestimates the MIZ extent in autumn. We estimate the potential impact of wave-induced fragmentation on ice dynamics, which the model suggests is important at short time scales and for some regions of the Arctic, like the Barents Sea, as sea ice mobility increases in the aftermath of storm events.

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MS34

From Micro to Macro in the Physics of Sea Ice and Climate

Sea ice exhibits composite structure on length scales ranging over many orders of magnitude. A principal challenge in modeling sea ice and its role in climate is how to characterize small scale structure and then find the effective behavior on larger scales relevant to climate and ecosystem models. The inverse problem of recovering small-scale parameters from bulk measurements is also of interest. Well tour recent advances, from the evolution of the fractal millimeter-scale brine inclusions and meter-scale melt ponds, to the geometry and homogenized dynamics of the marginal ice zone on the scale of the Arctic Ocean. Well also explore spectral representations in forward and inverse homogenization for two phase and polycrystalline composites, advection diffusion processes, and wave-ice interactions. Finally, considering these questions for sea ice leads us into other areas such as random matrix theory, Anderson localization, Morse theory, and topological data analysis.

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MS34

Towards Scale-Aware Sea-Ice Dynamics in the neXtSIM Model

Sea ice is a solid material that breaks and flows due to forcing from wind and ocean currents. Newly formed ice and ice in the marginal ice zone is thin and often highly broken up, while the ice in the central Arctic is thick and forms an essentially continuous sheet. This central pack breaks along narrow fracture lines, extending over hundreds of kilometres in patterns of clear velocity discontinuities and high deformation rates (shear and divergence). Investigations of satellite observations of sea-ice deformation have shown multi-fractality and scale invariance of the deformation rates, which has been challenging to model with traditional tools. In this talk, I will present the scaling analysis of sea-ice deformation and briefly discuss ideas for its origin. I will then discuss the current efforts in building a mathematical and numerical model to reproduce the observed behaviour. I will then present briefly the latest results of this work, done within the framework of the next-generation sea-ice model, neXtSIM. The model shows an exceptional ability to reproduce the observed deformation while running at the same resolution as that at which the fields were observed. I will also demonstrate that this new model is now suitable for use in large-scale models of sea ice, both on the regional and climate scale.

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MS35

Jutul - A Fully Differentiable Simulator for Porous Media Flow Written in Julia

The design of software that simulates any complex physical process is often a trade-off between performance, code readability and extensibility and generality. Programming in high level languages like Python and MATLAB allow for a read-eval-print loop (REPL) that produces code and prototype programs quickly, but getting good computational performance requires vectorization or extensions written in compiled languages. On the other hand, programming in lower level languages like Fortran, C or C++ yields much better computational performance, but the code can be complex for non-experts and the development process slowed by recompilation. Julia is a relatively new programming language that aims to bridge the gap between the two approaches for scientific computing. Jutul is an open source simulator framework written in Julia with a demonstrator application JutulDarcy for porous media flow that covers the usual flow physics (immiscible, multiphase miscible, compositional). The implementation is compact and highly efficient. In this talk, we: Discuss the design of the simulator and how this allows for highly efficient automatic differentiation Positive and negative aspects of developing simulation codes in Julia Examples of simulator performance Examples of the benefits of a fully differentiable simulator

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MS35

The OPM Flow Reservoir Simulator. Bridging Research and Industrial Usage

The OPM Flow open-source reservoir simulator has been developed through a long and close collaboration between industry and research. Various academic institutions and industrial partners in Europe and abroad are active developers. The aim is to develop a common research infrastructure that promotes industry-relevant research and development. Researchers get access to open datasets from industry and a tool that is robust, fast and reliable so that new methods and models can be tested on industry-relevant problems. Industry gets faster access to new development and research. The close collaboration with industry influences code development: choice of data structures, dependence on 3rd-party libraries and choice of numerical methods etc. Also field scale simulations involve solving a coupled system for the reservoir and the wells, strongly affecting linear solvers, preconditioners and parallelization. We will discuss some of the choices we have made and their consequences for performance and code complexity. In particular related to solving the coupled well-reservoir system and our discretization and automatic differentiation (AD) approaches. We will also touch on documentation, testing, how further development is organised between the parties and how the user community is involved.

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MS35

Software Design for an Open-Source Performance-Portable Multiphysics Simulator

Carbon capture and storage (CCUS) is a key component in efforts to reduce carbon emissions globally. The evaluation of CCUS candidate sites requires predictive simulation capabilities to assess site capacity and safety. To address the need for an open-source simulator capable of serving as the computational engine for CCUS evaluation workflows, we present an overview of the GEOS multiphysics simulation platform. We will present an overview of the discretization-data infrastructure, guidelines for construction and solution of single and coupled physics problems, and strategy to achieve reasonable levels of performance portability across hardware platforms. Additionally, the development process (coding standards, testing, verification, etc.) by which components of single and/or coupled physics capabilities are developed and merged into the main branch will be discussed. We will outline the approach to documentation, and the planned approach for user interaction. In addition to field scale CCUS simulations, GEOS is intended to serve as a research platform to investigate state-of-the art numerical methods and provide a transition plan for the evolution of those methods into hardened capabilities for field scale CCUS applications. Results of verification/validation problems with evaluations of GPU performance and weak scaling will be presented. Finally, the integration of the computational capabilities of GEOS into flexible python-based workflows will be discussed.

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MS36

Intrinsic Surface Vem for Vector Laplacian

We present an extension of the geometrically intrinsic formulation of the arbitrary-order Virtual Element Method (VEM) to vector-valued surface Laplacian on polygonal cells. The equation, written in covariant form using an appropriate local reference system, is discretized by the VEM approach. The knowledge of the local parametrization allows us to derive a two-dimensional VEM scheme for the contravariant components of the solution vector. The main advantage of the proposed formulation is that there is no need for additional projections or penalizations as the unknowns of the equation are objects that live intrinsically in the tangent space. We evaluate the method on several surfaces to show experimental convergence rates.

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MS36

Discontinuous Galerkin Methods on Polytopal Grids for Multiphysics Wave Propagation Problems

In this talk we present discontinuous Galerkin methods on polytopal grids (PolydG) for the numerical simulation of multiphysics wave propagation phenomena in heterogeneous media. In particular, we address wave phenomena in elastic, poro-elastic, and poro-elasto-acoustic materials. Wave propagation is modeled by using either the elastodynamics equation in the elastic domain, the acoustics equations in the acoustic domain and the low-frequency Biots equations in the poro-elastic one. The coupling between different models is realized by means of (physically consistent) transmission conditions, weakly imposed at the interface between the subdomains. For all models configuration, we introduce and analyse the PolydG semi-discrete formulation, which is then coupled with suitable time marching schemes. For the semi-discrete problem, we present the stability analysis and derive a-priori error estimates in a suitable energy norm. A wide set of two-dimensional verification tests with manufactured solutions are presented in order to validate the error analysis. Examples of physical interest are also shown to demonstrate the capability of the proposed methods.

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MS36

Nonnegative Moment Coordinates on Finite Element Geometries

We introduce new generalized barycentric coordinates (coined as moment coordinates) on 2D element geometries. This work draws on recent advances in constructing interpolants to describe the motion of the Filippov sliding vector field in nonsmoooth dynamical systems, in which nonnegative solutions of signed matrices based on (partial) distances are studied, further extended on specific hexaedra. For a finite element with n vertices (nodes) in $\mathbb{R}^d$, the constant and linear reproducing conditions are supplemented with additional linear moment equations to set up a linear system of equations of full rank n, whose solution results in the nonnegative shape functions. On a simple (convex or nonconvex) quadrilateral, moment coordinates and mean value coordinates are identical. Moment coordinates are valid on nonconvex quadrilaterals as well. Numerical examples are presented that affirm the properties of the shape functions and as verification tests, we demonstrate that the moment interpolant passed the patch test over two-dimensional finite element meshes. We also see how to extend moment coordinates on 3D element geometries.

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MS36

Weakly Imposing Boundary Conditions for Vem Discretisation of Linear Elasticity

In the framework of virtual element discretizations of linear elasticity, we address the problem of imposing nonhomogeneous Dirichlet and Neumann boundary conditions in a weak form, both on polygonal/polyhedral domains and on two/three dimensional domains with curved boundaries. We consider Nitsche's type methods. We prove that for the virtual element method, provided the stabilization parameter is suitably chosen, the resulting discrete problem is well posed, and yields convergence with optimal order on polygonal/polyhedral domains. On smooth two/three dimensional domains, we combine both methods with a projection approach similar to the one of Bramble et al. (1972). We prove that, given a polygonal/polyhedral approximation of the domain, an optimal convergence rate can be achieved by using a suitable correction depending on high order derivatives of the discrete solution along outward directions (not necessarily orthogonal) at the boundary facets. Numerical experiments validate the theory.

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MS37

Richards' Equation with Non-Local Root Water Uptake Modeling Plant Water Deficit

In this paper we present a novel way to mathematically frame the concept of *ecological memory* of plant water stress in the context of root water uptake in unsaturated flow equations. Inspired by recent eco-hydrological papers, we model the water content dynamics in a soil plant system by Richards equation with a non-local root water absorption term. In order to account for this memory term, an integral equation is defined, and sufficient conditions are provided for ensuring existence and uniqueness of its solution. Finally, tailored numerical methods are implemented, and numerical simulations are also provided.

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MS37

Challenges in Integrated Modelling of Terrestrial Systems in the Exascale Era

The Terrestrial Systems Modeling Platform (TSMP) is a scale-consistent, highly modular, physics-based, massively parallel, and fully integrated groundwater-vegetation-atmosphere framework for regional Earth system modeling. It integrates an atmospheric model (COSMO/ICON), a land surface model (CLM) and a hydrological model (ParFlow) via the OASIS3-MCT coupling library, as well as the PDAF data assimilation library. TSMP enables the simulation of processes across these three Earth system components, thus allowing to resolve feedbacks across the soil-vegetation-atmosphere continuum, for a wide range of applications from water resource assessments, to hydrometeorological extremes and climate change projections. The integrated modelling of terrestrial systems poses challenges in the formulation and parametrisation of surface and vegetation processes and in the effective coupling of fluxes and feedbacks. Moreover, the rapid evolution of computational technology creates challenges towards achieving efficient, performant, portable and sustainable computational implementations. In this contribution we present (i) the current and ongoing coupling approaches in TSMP working towards improved representation, in particular, of land surface processes, (ii) as well as the ongoing improvements in computational implementations of TSMP and its component models, leveraging on the exascale era of supercomputing, in turn enabling more ambitious modeling strategies and applications.

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MS37

Micromechanical Analysis of the Effective Stiffness of Poroelastic Composites

Within this work we investigate the role that the microstructure of a poroelastic material has on the resulting elastic parameters. We are considering the effect that multiple elastic and fluid phases at the same scale (LMRP [Miller, L., and R. Penta. Continuum Mechanics and Thermodynamics 32.6 (2020): 1533-1557.]) have on the estimation of the materials elastic parameters when compared with a standard poroelastic approach. We present a summary of both the LMRP model and the comparable standard poroelastic approach both derived via the asymptotic homogenization approach. We provide the 3D periodic cell problems with associated boundary loads that are required to be solved to obtain the effective elasticity tensor for both model setups. We then perform a 2D reduction of the cell problems, again presenting the 2D boundary loads that are required to solve the problems numerically. The results of our numerical simulations show that whenever investigating a poroelastic composite material with porosity exceeding 5% then the LMRP model should be considered more appropriate in incorporating the structural details in the Youngs moduli E_1 and E_3 and the shear C_44. Whenever the porosity exceeds 20% it should also be used to investigate the shear C_66. We find that for materials with less than 5% porosity that the voids are so small that a standard poroelastic approach or the LMRP model produce the same results.

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MS38

Ensemble Data Assimilation for Complex Multiphysics Models

Based on the formulation and notation from the recent open-access book, Data-Assimilation Fundamentals, A Unified Formulation of the State and Parameter Estimation Problem by Evensen et al. (2022), (`https://link.springer.com/book/10.1007/978-3-030-96709-3`) this presentation will discuss ensemble data assimilation for nonlinear physical models. We will discuss using iterative methods to handle "weak" nonlinearities in the model and measurement operators. Notably, the iterative ensemble smoothers approximately sample the posterior Bayesian, and they efficiently solve high-dimensional parameter and state estimation problems. These methods are in operational use in fields like weather prediction and petroleum reservoir management. We will illustrate using iterative ensemble smoothers for estimating poorly known high-dimensional model parameters and model controls in some examples involving reservoir engineering and pandemic models.

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MS38

Data Assimilation and Hydro-Mechanical Models in Real-World Reservoir Simulations

The awareness about the critical importance of dealing with uncertainty in numerical models is spreading over an increasing number of application fields, including geomechanics for energy resources. Sources of uncertainty are related for instance to the mathematical law governing the rock behavior, the geomechanical parameters and the geological nature of the field. By combining hydro-mechanical models with successive steps of data assimilation, we define a novel comprehensive model for the management of active reservoirs, which automatically integrates real measurements and progressively reduces the prediction uncertainties by a continuous training in time. In this communication, we present a real-world application of the proposed approach for land subsidence prediction over an off-shore hydrocarbon reservoir in Italy.

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MS38

Estimating Fracture Apertures from Push-Pull Data in Enhanced Geothermal Systems via Ensemble-Based Data Assimilation

Geothermal energy extraction often targets fractured rock masses. If so, a detailed characterisation of the fractures is essential because of their importance for flow and transport. Fracture aperture and its variation among fractures must be characterised to reliably predict performance and assess risks. Aperture, however, is a dynamic property that is difficult to measure in situ so that estimates are always associated with large uncertainties. In reservoir engineering, ensemble-based data assimilation is widely used for history matching and uncertainty reduction. In this work, we apply an ensemble smoother with multiple data assimilation (ES-MDA) to improve estimates of fracture aperture in discrete fracture and matrix geothermal reservoir models. To illustrate the application of ES-MDA to dynamic data from push-pull tests, a synthetic 3D geothermal reservoir with a moderate number of fractures is considered. We assume that the geometry of open fractures is known, and their apertures are the only unknown model parameters. In the push-pull tests, cold water with a non-sorbing tracer is injected and retrieved from the same well. Back-flow temperature and potential tracer loss inform the ES-MDA that updates fracture apertures iteratively. This flow-physics based data assimilation method is shown to reduce model uncertainty significantly, especially for fractures that connect directly to the well.

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MS39

Numerical Modelling of Waves Impacting Rigid and Flexible Structures

Wave-structure interactions (WSI) are complex phenomena in a range of coastal and offshore applications such as oil and gas rigs, offshore wind turbine platforms, breakwaters, dams and wave energy converters. These structures experience stresses and deformations under wave loading resulting in damage or even failure in extreme cases. The present study focuses on the modelling of waves impacting rigid and flexible structures with the numerical model solids4foam. Solids4foam couples a fluid and solid solver with a partitioned approach, employing a Finite Volume Method discretisation for both domains. After validation with analytical, laboratory and numerical results, solids4foam was used to model a range of WSI phenomena. Tsunamis impacting dams of several inclinations were simulated first. Tsunamis were modelled as idealised waves, e.g. Stokes, cnoidal and solitary waves, to represent a range of waves generated by earthquakes, landslides and icebergs. A range of linear and solitary waves impacting plates of different stiffnesses were then investigated. Plates located either offshore or onshore were employed mimicking a range of real applications. Novel insight into WSI effects is provided along with various empirical and semi-empirical prediction equations for pressures, forces and deflections. These findings are hoped to enhance the physical understanding, support the design and optimise the modelling of WSI.

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MS39

Probabilistic Landslide Tsunami Estimation in the Makassar Strait, Indonesia, Using Statistical Emu-

lation

This paper presents a significant advancement in the understanding of tsunamigenic landslide hazard across the length of the Makassar Strait in Indonesia. We use statistical emulation across the length of the continental slope to conduct a probabilistic assessment of tsunami hazard on a regional scale, across 14 virtual gauges. Focusing on the potential maximum wave heights from possible tsunamigenic landslide events, we generate predictions from Gaussian Process Emulators fitted to input-outputs from 50 training scenarios. We show that most probable maximum wave heights in the majority of gauges are between 1 and 5 m, with the maximum predicted heights reaching values of up to 10 m on the eastern coast, and up to 50 m on the western coast. We also explore the potential use of Gaussian Multivariate Copulas to sample emulator prediction input values to create a more realistic distribution of volumes along the continental slope. The novel use of statistical emulation across a whole slope enables the probabilistic assessment of tsunami hazard due to landslides on a regional scale. This area is of key interest to Indonesia since the new capital will be established in the East Kalimantan region in the Western side of the Makassar Strait.

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MS39

Uncertainty Quantification When Using Integrated Physics Driven and Data Driven Models

Complex physical systems like those from large scale mass flows from debris flows and tsunamis requires physics and data driven models orchestrated carefully to determine the potential impact. Analysis of the uncertainty in these computations requires novel methodology we will discuss in this talk.

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MS40

Development and Verification of a Framework for Coupled Thermal, Hydrologic, and Biogeochemical Modeling of Arctic Permafrost

Many permafrost modeling studies have focused on coupled thermal dynamics and structural property evolution within Arctic permafrost under changing environmental conditions. Of growing concern is not only the structural impact of thawing permafrost but also the potential for permafrost thaw to significantly affect CH4 and CO2 greenhouse gas (GHG) fluxes. In particular, CH4 is understood to be an increasingly important component of global GHG emissions, however current global climate models do not adequately account for CH4 sourced from permafrost soils. We present the development of an open source, high performance software framework for modeling coupled thermal-hydrologic and biogeochemical processes affecting GHG fluxes from Arctic soils, with emphasis on current model verification efforts and ecotype-based stylized model design. Development of this framework is being pursued by a multi-institutional team as part of the Coupled Hydro-thermo-biogeochemical modeling For Predicting Arctic Carbon Emissions (CH4PACE) project. We begin our project with a focused study in Alaska and aim to create a data driven, flexible framework for modeling permafrost which includes hydrological, thermal, and biogeochemical processes. Our ultimate goal is to use the model to create probabilistic simulations to provide source/sink terms of CH4 and CO2 that are directly integrated into global climate models. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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MS40

Development of the Arctic Coastal Erosion Model with a Demonstration at Drew Point, AK

The ACE (Arctic Coastal Erosion) Model is a multi-physics numerical tool that couples oceanographic and atmospheric conditions with a terrestrial permafrost domain to capture the thermo-chemo-mechanical dynamics of erosion along permafrost coastlines. It is based on the finite-element method and solves the governing equations for conservation of energy (heat conduction with phase change), and conservation of linear and angular momenta using a plasticity material model. Oceanographic and atmospheric boundary conditions force evolution of a permafrost environment, consisting of porous media made of sediment grains and pore fluid. An oceanographic modeling suite (external software packages) produces time-dependent water level, temperature, and salinity boundary conditions for the terrestrial domain. Atmospheric temperature is obtained from the ECMWF Reanalysis v5 (ERA5) dataset. Driven by these boundary conditions, 3-D solutions of temperature, stress, and displacement develop in the terrestrial domain in response to the plasticity model that is controlled by the frozen water content. Material is removed when the stress or strain within an element exceeds the yield strength or strain limit of the material and is followed by grid adaptation that captures the new geometry. This modeling approach enables failure from any allowable deformation (e.g., block failure, slumping, thermal denudation) and can treat erosion behavior over single events, seasonally, or over several years.

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MS40

Numerical Modeling of Viscous-Plastic Sea-Ice Dynamics

Subject of this talk are the mathematical challenges and the numerical treatment of large scale sea ice problems. The model under consideration goes back to Hibler (A dynamic thermodynamic sea ice model, J. Phys. Oceanogr., Hibler 1979) and is based on a viscous-plastic description of the ice as a two-dimensional thin layer on the ocean surface. In the first part of this talk we discuss the model in order to find a suitable presentation for applying numerical analysis and modern approximation techniques. The second part focuses on the presentation of new numerical methods to discretize the strongly nonlinear equation in space. In last part of the talk we discuss the limits of the model and outline new approach to improve the representation of sea ice in climate models.

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MS40

Numerical Modeling of Permafrost Thermal Dynamics in Arctic Lake-Soil Systems Using Amanzi-Ats

Permafrost degradation is observed to increase rapidly in Arctic coastal regions due to permafrost warming. Increases in air temperature is the primary direct driver of permafrost warming, but frequent coastal flooding has been recognized as another important driver indirectly contributing to permafrost warming. However, the impact of coastal flooding on permafrost has not been tested and remains poorly understood. Our goals are to 1) understand permafrost hydro-thermal dynamics under floods and 2) develop new capability to simulate arctic lake and permafrost thermal dynamics. We consider a coupled one-dimensional model of snow-lake-soil system with variable water body depth. The temperature distribution in the lake (with or without ice) is calculated by means of a heat diffusion equation in the scaled coordinate system to account for variability in the depth. The soil is a coupled model of heat equation for the temperature and Richards equation for the water content. Finally, we use the surface energy balance equation to model the snow layer. The numerical discretization and coupling of the physical processes are performed using the Amanzi-ATS software infrastructure. For model verification we compare the results of Amanzi-ATS simulations for three different lakes in Alaska with the seasonal observation data for the surface temperature and the depth of the snow and ice layers.

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MS41

Direct Numerical Simulation of Mixing and Fronts in a Porous Medium Column

We use high resolution numerical direct numerical simulations to study flow and transport in a full length porous column, solving the Navier-Stokes and advection-diffusion equation to fully resolve all processes at pore scale. The data is used to take a very close look at interfacial and mixing processes at unprecedented resolution, enabling us to accurately track mixing interfaces, quantify incomplete mixing and reactions and study boundary effects to gain a deeper understanding of the origin of anomalous behaviors that cannot currently be measured in laboratory experiments.

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MS41

A Latice-Boltzmann Model for Paravascular Flow Simulations with Pulsating Vessel Walls

Optimal drug delivery in the brain, stroke, and neurodegenerative disorders like Alzheimer's disease are mainly affected by the solute transport in the brain. The transport is facilitated by the circulation of cerebrospinal fluid and interstitial fluid around the brain. Mathematical modeling and computational analysis offer tools to understand and assess the complex resulting phenomena. Current mathematical models consider the flow in the porous paravascular tissue with prescribed pulsation of the vessel wall, which is taken from medical data, see e. g. [C. Daversin-Catty, et al., The mechanisms behind perivascular fluid flow, 2020], [R. T. Kedarasetti, et al., Arterial vasodilation drives convective fluid flow in the brain: a poroelastic model, 2022]. In contrast, we developed a computational model for the coupled processes of blood flowing through an elastically deformable vessel embedded in the porous paravascular tissue where the cerebrospinal fluid flows. We base our simulations on the Lattice-Boltzmann Method to solve all coupled equations in a monolithic approach using the generalized Navier-Stokes equation together with an elastic membrane equation. Further (long-term) goals are the use of geometries reconstructed from actual MRI-scans and boundary conditions being obtained from one-dimensional circulatory network simulations [M. Fritz, et al., A 1d-0d-3d coupled model for simulating blood flow and transport processes in breast tissue, 2022.].

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MS41

An Overview of Results on Evolving Micro-Structures in Porous Media Flow

In this talk, we shall investigate a system of reaction-diffusion equations modeling multi-species transport phenomena in a porous medium. We incorporate our model with crystal dissolution and precipitation on the interfaces of the solid parts of the porous medium which leads to an evolving microstructure. Recently, several techniques have been proposed to deal with the evolving microstructures such as level set method, phase-field models, the transformation of the evolving domain to a fixed one, etc. We shall look into an overview of all these methods and use them to tackle our model. We will also motivate the concept of optimal control problem for our model and pair it with the existing results on flow in porous media.

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MS41

Micro-Macro Models for Mineral Dissolution

Porous media naturally exhibit a heterogeneous structure including two different spatial scales. (Periodic) homogenization has been successfully applied to bridge these scales and to arrive at macroscopic (upscaled) models, which only keep the microscopic information by means of a decoupled computation of effective parameters on a so-called unit cell. However, the situation becomes more involved, if competing minerals dissolve and precipitate and consequently dynamically alter the porous mediums structure and its bulk properties. For such a situation, we derive an effective model by formal two-scale asymptotic expansion in a level-set framework. The resulting macroscopic equations (reactive flow and transport equations) and the equations posed at the unit cells are fully coupled. Moreover, the underlying geometry of the unit cells is changing dynamically in space and time and so do the effective hydrodynamic parameters porosity, reactive surface, diffusion, and permeability. We present numerical simulations with application to dissolution of calcite and dolomite and discuss their acceleration by means of neural networks or statistical parameter estimation methods.

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MS42

Robust and Scalable Solvers in Nonlinear Poroelasticity

This talk will address the numerical approximation of fully nonlinear poroelastic models, allowing for large deformations in a variety of different physical contexts but with particular attention to biological and soft tissue modeling. These models possess two main difficulties beyond the standard ones from Biot equations: i) the stress response of the elastic material is nonlinear, and most importantly non-convex; ii) pressure is no longer a variable, but is instead obtained through constitutive modeling. We will see how standard splitting-schemes can be adapted to handle many scenarios, such as total- and quasi-incompressibility of the solid phase, and how the preconditioner obtained comes into play in the context of Newton solvers for the model problem. The robustness of this approach will be validated with different test cases in High Performance Computing infrastructures.

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MS42

Higher Order Space-Time Finite Element Methods for Dynamic Poroelasticity

Space-time finite element methods feature the natural construction of higher order discretization schemes for coupled systems of partial differential equations [M. Bause et al., Convergence of a continuous Galerkin method for mixed hyperbolic-parabolic systems, Comput. Math. with Appl., submitted (2022), pp. 1-24; arXiv:2201.12014]. They offer the potential to achieve accurate results on computationally feasible grids and preserve the structure of the continuous problem on the discrete level. We present, analyse and compare families of tailored space-time finite element methods for two- and multi-field formulations of the dynamic Biot system, including a first-order in space and time system based on Picards solution theory. Error estimates and benchmark studies for the numerical evaluation of the model representation and finite element types in space and time are addressed. Finally, the efficient solution of the algebraic systems with block structure of growing complexity for higher polynomial degrees is considered. Geometric multigrid preconditioning using local Vanka smoother is suggested [M. Anselmann, M. Bause, A geometric multigrid method for space-time finite element discretizations of the NavierStokes equations and its application to 3d flow simulation, ACM Trans. Math. Softw., submitted (2021), pp. 1-27; arXiv:2107.10561].

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MS42

Gradient Flow Structures of Multiphase Poroelasticity and Splitting Schemes

Multiphase poromechanics constitutes the two-way coupling of multiphase flow and geomechanics in deformable porous media. Strongly coupled processes governed by multiphase poromechanics are relevant in applications such as CO2 sequestration, geothermal energy, and many more. The resulting model is highly nonlinear, possibly degenerate and strongly coupled. Thus, robust and efficient numerical solution strategies are required for effective numerical simulations. Numerical solvers have been well understood for linear poromechanics, being often based on stabilized iterative schemes (often also formulated as preconditioners). A sound mathematical understanding in the presence of multiphase flow has been however lacking. In this talk, we investigate gradient flow structures of the coupled mathematical model for multiphase poromechanics and discuss iterative solvers utilizing this structure, i.e., aiming at decreasing a suitable energy functional in order to converge robustly.

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MS42

Structure-Preserving Discretization and Robust Preconditioning Techniques for Poromechanics

In this talk we discuss homogenized multicompartmental poromechanics models arising from generalization of Biot's model of consolidation with a focus on applications in biomechanics. We consider quasi-static as well as dynamic systems and derive optimal error estimates and fully parameter-robust operator preconditioners for a family of physics-oriented discretizations, i.e., taking into account the conservation of mass as well as of momentum and energy using an $H(\mathrm{div})$-conforming ansatz in space and continuous Galerkin-Petrov (cGP) methods in time. The analysis we present exploits a recently developed abstract framework to establish the parameter-robust inf-sup stability of perturbed saddle-point problems from a small inf-sup condition similar to the famous Ladyzhenskaya-Babuška-Brezzi (LBB) condition and the other standard assumptions in Brezzi's theory, cf. [Hong, Q., Kraus, J., Lymbery, M., and Philo, F., A new practical framework for the stability analysis of perturbed saddle-point problems and applications, Math. Comp. 92 (2023), 607-634].

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MS43

An Optimization Based Domain Decomposition Strategy for 3D-1D Coupling on Non-Conforming Meshes

In this talk a new framework for 3D-1D coupling is proposed, based on a well posed mathematical formulation and ending up in a method which is highly robust and flexible in handling geometrical complexities. Two scenarios are considered: in a first case, the problems are coupled by imposing flux conservation and solution continuity, thanks to a three-field domain decomposition strategy; a second approach allows instead for discontinuous solutions, with the exchanged flux being proportional to the jump of the solution itself. The resulting problems are solved in a PDE-constrained optimization framework: a cost functional mimicking the error committed in the fulfillment of matching conditions is introduced and minimized subject to the 3D and 1D equations. Under this approach no mesh conformity is required, so that the 3D and the 1D domains can be meshed separately. An iterative solver is proposed for both approaches, together with ad-hoc built preconditioners.

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MS43

Efficient Solvers for Coupled Mixed-Dimensional Problems

Systems describing interaction between diffusive processes in the 3d/2d bulk domain and on an embedded manifold of codimension 1or 2 arise as models in computational biomechanics or neuroscience as well as Riesz map operators in preconditioning various coupled multiphysics problems. In these applications the requirements for robustness with respect to the discretization and model parameters present a challenge for design of efficient solution algorithms. In this talk we address this issue by developing several robust preconditioners for Krylov solvers. In particular, approaches based on (i) non-overlapping domain decomposition, (ii) tailored multigrid methods targeting the low rank perturbation term and (iii) block diagonal preconditioners utilizing fractional operators on the coupling manifold will be discussed.

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MS43

Analysis of 1D-3D Nonlinear Parabolic Models in a Hilbertian Framework

In this talk, we present the analysis of time-dependent coupled 1D-3D nonlinear models. The coupling lies in the source term. For the equation driving the flow in the 3D domain, the source is assumed to be given by a Dirac measure along a line. Models of this type have been used e.g. to simulate fluid flow between well and reservoir or blood flow in vascularized tissue. For numerical purposes, inclusions in the medium are represented by 1D structures, giving rise to the aforementioned 1D-3D model. In particular our aim is to prove the well-posedness of nonlinear parabolic equations such as Richard's equation or filtration (porous medium) type models in a Hilbertian framework. This specific functional setting allows us to apply simple finite element techniques and hope to recover optimal convergence rates using graded meshes (i.e. meshes that are refined progressively approaching the 1D inclusions). Hence, after explaining the motivations of this work, we present the functional setting of weighted Sobolev spaces (with weights depending on the distance to the one dimensional inclusion). We then discuss the literature and explain the difficulties arising in the parabolic case. We show our main result concerning well-posedness of 1D-3D parabolic models with Dirac line sources. We conclude the presentation with some numerical simulations.

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MS44

Combining Data Assimilation and Machine Learning to Improve Dynamical Models

Climate models are numerical implementations of dynamical systems expressed as partial derivative equations representing the evolution of the Earth System (e.g. ocean, atmosphere). They are used to provide projections/predictions of the Earth climate. Two major sources of uncertainty plague these predictions: the system's initial condition is generally imperfectly known, and the models themselves have large errors because many key processes are either unknown or unresolved and thus parameterized. Both these uncertainties can be tackled by properly using data. Observations of the atmosphere or the ocean are noisy, sparse, and heterogeneously distributed, but, with the emergence of satellite data, high-resolution observations are becoming massively available. Data assimilation (DA) has been widely used to blend observations and dynamical models, in particular, to estimate the initial condition of the forecast in the numerical weather community. Progress in DA has contributed a lot to improving forecasts, but only to a limited extent to improving the prediction model itself. In this presentation, we will introduce how we can leverage machine learning and data assimilation to correct the model error and thus improve the forecast. The general concept is to learn the model error by a machine learning algorithm and to produce a hybrid model, merging a physical core with a data-driven component. This concept will be demonstrated in practical applications from the Earth system.

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MS44

Online Model Error Correction with Neural Networks – Towards An Implementation in the Ecmwf Data Assimilation 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 those 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 state estimate is computed. Online approaches 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 a two-scale Lorenz system and a two-layer two-dimensional quasi geostrophic model. Preliminary results shows the potential of incorporating DA and ML tightly, and pave the way towards its application to the Integrated Forecast System (IFS) used for operational Numerical Weather Prediction at ECMWF.

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MS44

Towards Ultra-High Resolution - Including Nonhydrostatic Dynamics in Icon-O

We develop a conservative low-order method to discretize the three-dimensional Euler and Navier-Stokes equations on anisotropic approximation spaces. The discretization preserves important discrete equivalents of continuous conservation laws. The natural approximation space on these anisotropic approximation spaces contains a spurious mode that arises from the imbalance of the degrees of freedom of the horizontal grid. This mode is filtered out by a projection operator that is integrated in the numerical scheme in a manner that is compatible with the discrete conservation laws. This work is an extension of the authors work on the hydrostatic Boussinesq equations of ICON-O towards non-hydrostatic equations and their application in ocean modelling. Simulations based on a telescoping capability are presented towards ultrahigh-simulation in global ocean modelling

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MS44

High Order Sea-Ice Modeling with neXtSIM_DG

Simulation of sea ice dynamics consumes a significant fraction of the computational time in coupled climate models. Moreover, the ice models, i.e., e.g., the rheology, are not of a physical quality as, e.g., the models describing the athmosphere and ocean. The most frequently used model is the viscous-plastic model which goes back to Hibler as well as variants of it. However, this model is difficult to approximate numerically due to its strong nonlinearity. Furthermore, simulation results do not agree well with observations in some aspects. We describe a software framework for the simulation of sea ice dynamics using modern high-order numerical approximation techniques. On the one hand, the implementation is efficient and builds on a clearly structured data management. On the other hand, the implementation is flexible and allows the consideration of different ice rheologies.

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MS45

Defining Climate by Means of an Ensemble

We study the suitability of an initial condition ensemble to form the conceptual basis of defining climate. We point out that the most important criterion is the uniqueness of the probability measure on which the definition relies. We first propose, in harmony with earlier work, to represent such a probability measure by the distribution of ensemble members that have converged to the probability density of the natural probability measure of the so-called snapshot or pullback attractor of the dynamics, which is time dependent in the presence of external forcing. Then we refine the proposal by taking a density that is conditional on the (possibly time-evolving) state of system components with time scales longer than the horizon of a particular study. We discuss the applicability of such a definition in the Earth system and its realistic models, and conclude that micro initialization from observations in slower system components perhaps provides the practically relevant probability density after a few decades of convergence. However, the absence of sufficient time scale separation between system components or regime transitions in slower system components might preclude uniqueness, at least in certain subsystems, and time evolution in slower system components might induce unforced climate changes, leading to the need for targeted investigations to determine the forced response. We propose an initialization scheme for studying all these issues in Earth system models.

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MS45

Simulation of Extreme Events in Climate Models with Rare Event Algorithms

The study of extreme events is one of the main areas of application of numerical climate models. Events like heat waves, floods or wind storms, have huge impacts on human societies, and a better understanding of their statistics and predictability is crucially important. Studying extreme and rare events on a robust statistical basis with complex climate models is however computationally challenging, as very long simulations and/or very large ensembles are needed to sample a sufficient number of events. This problem can be tackled using rare event algorithms, numerical tools dedicated to reducing the computational effort required to sample rare events in numerical models. These methods typically take the form of genetic algorithms, where a set of suppression and cloning rules is applied to members of an ensemble simulation, in order to oversample trajectories leading to the events of interest. We show recent applications of these methods to the simulation of heat waves and warm summers in the Northern hemisphere. We show how a rare event algorithm allows to efficiently sample events characterised by persistency of high regional surface temperatures, and we analyse the emergence of atmospheric teleconnections during the events. We then present applications to extremes of Arctic sea ice reduction and weakening of the Atlantic Meridional Overturning Circulation, and we discuss how these results open the way to further applications to a wide range of problems.

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MS45

Ensembles of Exploration

Can we design ensembles to aid our escape from model land? Traditional ensemble simulations explore flat envelopes within model-land. Ensembles of exploration are designed to advance our understanding of the system and increase the fidelity of model-based insights in the real world, while exposing limits on what can be exported from model-land honourably. Fundamental constraints on the utility of ensemble simulation are discussed in a nonlinear dynamical systems framework. Structural model error disqualifies all common probability interpretations; lack of structural stability is sufficient, but not necessary. Parameter selection, when no “true” parameter value exists, is noted. [Berger, J & Smith, L (2019) ‘On the statistical formalism of uncertainty quantification,’ Ann Rev Stats, 6. Frigg, R. et al (2015) ‘An assessment of the foundational assumptions in high-resolution climate projections’, Synthese] It is argued that a more uniform, transparent approach to quantifying nontrivial skill [Smith, L et al (2015) ‘Towards improving the framework for probabilistic forecast evaluation’, Climatic Change], clarifying the relevance of model output in each given application, and publicising the lead times at which ensemble-based outputs are likely to prove misleading are essential in all science; climate science in particular. Focusing on ensembles of exploration explicitly will speed achievement of these goals and achieve key insights for climate science in application.

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MS45

A Low-Dimensional Dynamical Systems Approach to Climate Ensemble Design and Interpretation

Earth System Models (ESMs) are complex, highly nonlinear, multi-component systems described by large number of differential equations. They are used to study the evolution of climate and its dynamics, and to make projection of future climate at both regional and global levels which underpins climate change impact assessments such as the IPCC report. These projections are subject to several sorts of uncertainty due to high internal variability in the system dynamics, which are usually quantified via ensembles of simulations. Due to their multi component nature of such ESMs, the emerging dynamics also contain different temporal scales, meaning that climate ensembles come in a variety of shapes and sizes. However, our ability to run such ensembles is usually constrained by the computational resources available, as they are very expensive to run. Hence, choices on the ensemble design must be made, which conciliate the computational capability with the sort of information one is looking for. One alternative to gain information is to use low-dimensional climate-like systems, which consists of simplified, coupled versions of atmosphere, ocean, and other components, and hence capture some of the different time scales present in ESMs. This approach allows one to run very large ensembles, and hence to explore all sorts of model uncertainty with only modest computational usage. In this talk, we discuss this approach in detail, and illustrate its applicability with a few results.

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MS46

Comparison of Flow-Mechanics Iterative Coupling Schemes for Fractured Poroelastic Media

The efficient coupling of subsurface flow and reservoir geomechanics is an essential tool for obtaining accurate results when modeling multiphsyics scenarios such as wellbore stabilities, hydraulic fracturing, and pore-predictions.

This becomes more important in the case of fractured reservoirs requiring accurate underlying fractured poro-elastic models. In this work, we compare the accuracy and efficiency of two well-known iterative coupling schemes for coupling flow and geomecahnics, mainly the fixed-stress split scheme and the undrained split scheme. In the fixed stress split scheme, the flow problem is solved first, and the mean total stress is kept fixed during the flow solve. In contrast, in the undrained split scheme, the mecahnics problem is solved first, and the fluid content of the medium is kept fixed during the mechanics solve. We first show the extensions of both schemes to fractured poro-elastic media theoretically. The convergence of the two extended scheme will be established and linear rates of convergence, represented by the associated contraction coefficients, will be compared for both schemes, along with the underlying derived conditions constraining the convergence of the corresponding scheme. Time-permitting, the numerical efficiency of both schemes will be compared in terms of the number of iterative coupling iterations per time step.

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MS46

HPC Multiphysics Simulation of Co2 Geological Storage

Safe and efficient operation of CO_2 geological storage projects requires numerical simulation of a multi-physics problem in which compositional multiphase flow and transport are tightly coupled with the porous medium deformation. To simulate these processes, one needs to solve a set of coupled, nonlinear, time-dependent partial differential equations (PDEs) governing the conservation of mass of each component and linear momentum of the solid-fluid mixture. We present a scalable fully-implicit framework based on a displacement/pressure/component density formulation. The discrete displacement field is approximated using nodal interpolation. Pressure and component densities are assumed cell-wise constant, with interface pressure also present if a hybridization strategy is chosen. A Newton-Krylov approach is used to advance the solution in time, with a finely-tuned multigrid reduction (MGR) preconditioner introduced to accelerate convergence. The solver is implemented in an open-source, exascale-compatible, research-oriented simulator for modeling fully coupled flow, transport and geomechanics in geological formations. Numerical results are presented to illustrate performance and robustness of the proposed solver on a variety of challenging test problems, including realistic field cases.

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MS46

A Sequentially Coupled Fixed Stress Algorithm for Black Oil Flow in Poroelastic Media

We develop a novel computational model for solving black oil flow in poroelastic media based on the sequentially coupled fixed stress algorithm framework. The extended flow equations, describing the movement of the aqueous, oleic, and gaseous phases, incorporate new complex features associated with transient porosity and are rewritten in a proper Lagrangian formulation. The fluxpressure system is linearized by a Newton scheme and discretized by a mixed-hybrid finite element method with the lowest order Raviart Thomas element. The elasticity subsystem with the additional body force associated with the pressure gradient is also discretized by a mixed formulation based on decomposing the effective stress into spherical and deviatoric components. The system of conservation laws for the saturations is discretized by an extended version of a central-upwind finite volume scheme. The potential of the computational model is illustrated in numerical simulations of water-flooding problems in poroelastic media.

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MS46

Impact of Compacting Reservoirs on Flow Potential of Fractured Porous Layers in Overburden Formations

Formations in the overburden of hydrocarbon fields with flow potential needs to be plugged during future plug and abandonment (P&A) operations. It is essential to assess the flow potential of porous layers in the overburden. In this context, fractured formations with weak mechanical properties are, among others, of primary concern due to the potential alteration of their flow properties caused by deformation above depleted and compacting reservoirs. The focus in the past research has been on the effect of far field stress on fracture apertures. It is still unknown how much the deformation of an underlying reservoir during hydrocarbon production can affect the flow potential of fractured formations in overburden. This study mainly aims to answer this question. Moreover, we explore the mechanisms controlling the changes of flow potential in production phase. For this purpose, a fracture model has been proposed to consider empirical formulations of Barton-Bandis in ABAQUS. Then through conducting several simulations utilizing a 2D discrete fracture and matrix (DFM) model, the effect of both underlying deformation and the direct production from target formation on flow potential of overburden is investigated. It is shown that dilation caused by underlying deformation has a key role in the dynamic of aperture distribution controlling the flow potential towards wells.

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MS47

Model Flexibility and Performance Portability for Extreme-Scale Earthquake Simulations with SeisSol

SeisSol (www.seissol.org) is an earthquake simulation software that offers modelling flexibility for simulating seismic wave propagation in various media (elastic, viscoelastic, elastic-acoustic, poroelastic) and with different rupture laws. It has been optimised for a wide range of CPU and GPU architectures, and has achieved beyond-petascale performance on various supercomputers. Achieving portable performance on these architectures and for the entire range of models poses a substantial challenge for the code design, which is met by a code generator approach. The DSL and code generator YATeTo ("Yet another tensor toolkit") offers an abstraction layer that simplifies the implementation of numerical schemes, applies various algorithmic optimisation steps and employs hardware-optimized backends for high-performance kernels. We will report on recent results on various supercomputers with CPU and GPU architectures, where the use cases include simulations of seismo-acoustic nuisance patterns from induced earthquakes, coupled simulation of tsunami-earthquakes events or dynamic rupture simulation on complex fault geometries.

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MS47

Performance Improvements in Multilevel Spectral Domain Decomposition

Multilevel spectral domain decomposition methods are provably robust and efficient methods that can be used as preconditioners as well as multiscale methods when solving heterogeneous elliptic partial differential equations. With respect to high performance computing they offer plenty of opportunities for performance improvements. In this talk we will mainly focus on performance improvements in the (very costly) setup phase which involves the solution of generalized eigenproblems and the Galerkin projection of matrices.

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MS47

Efficient Hybrid-Parallel Solvers for Subsurface Flow Problems

Modern computing clusters and super computers consist of (usually multiple) CPUs with an increasing number of processor cores. Parallelisation based on MPI only is not efficient on these architectures, as it requires to store an overlap on parallel meshes (which can be significant for higher-order FEM-spaces). Furthermore, strong preconditioners are necessary for the huge sparse linear-equation systems involved. Algebraic Multigrid Solvers have proofed to be very efficient for subsurface flow problems. A hybrid-parallel realization of AMG allows a more flexible coarsening and reduces communication costs. In this talk we present a highly efficient solver library exploiting vectorization, expression templates, multi-precision and multi-threading to obtain an optimal performance and a high memory efficiency on a single shared-memory node, while allowing scalability to large clusters with MPI. Used in combination with DUNE PDELab it will facilitate the solution of extremely large subsurface flow problems on current supercomputers. We present high-resolution steady-state diffusion problems as test cases.

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MS47

Um-Bridge: Universal UQ/model Interface, UQ Benchmark Library and Turn-Key HPC in the Cloud

This talk presents UM-Bridge, a language-agnostic software interface for coupling any simulation code to any Uncertainty Quantification (UQ) software (and, to some degree, optimization and model order reduction). At the time of writing, easy to use integrations for C++, Python, R, MATLAB, and several established software packages like PyMC, MUQ and QMCPy are available. Inspired by microservice architectures, UM-Bridge enables containerization of models. This allows UM-Bridge to provide the, to our knowledge, first library of ready-to-use UQ benchmark problems. Further, UM-Bridge provides a kubernetes configuration that immediately allows running any containerized UM-Bridge model in cloud environments at HPC scale. On the UQ side, software complexity for HPC-scale applications is significantly reduced as well, as the kubernetes configuration takes care of most issues when controlling many parallel model instances. Finally, we demonstrate the effectiveness of the approach at the example of an HPC-scale UQ application.

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MS48

Mixed Fem for Rotation-Based Poroelasticity

We present a mixed finite element method for Biot poroelasticity which is based on i) the formulation of linear elasticity as a weighted vector Laplace problem and ii) the introduction of the solid rotation, leading to a four field formulation of poroelasticity for the unknowns: displacement, rotation, pressure and Darcy flux. The system is then discretized using conforming mixed finite element spaces, and we prove well posedness and convergence for two choices of such spaces. By a choice of quadrature formula common to multipoint flux mixed FEMs, the additional variables rotation and flux can be locally eliminated by static condensation, leading to a two-fields formulation that, notably, can be approximated with the lowest order Raviart Thomas elements for displacement and pressure, thus, with a very low number of DOFs. Moreover, one can prove that some quantities are completely unaffected by the hybridization, whereas the others converge to the solution of the full discrete problem. Thanks to the definition of a parameter weighted norm a block diagonal preconditioner can easily be defined for the four fields problem. Numerical results show the expected convergence, and robustness of the preconditioner for different choices of the parameters. Moreover, with a suitable reformulation of the boundary condition the method is successfully applied to the well known Mandel's test case.

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MS48

A Space-Time Multiscale Mortar Mixed Finite Element Method for Parabolic Equations

We develop a space-time mortar mixed finite element method for parabolic problems. The domain is decomposed into a union of subdomains discretized with non-matching spatial grids and asynchronous time steps. The method is based on a space-time variational formulation that couples mixed finite elements in space with discontinuous Galerkin in time. Continuity of flux (mass conservation) across space-time interfaces is imposed via a coarse-scale space-time mortar variable that approximates the primary variable. Uniqueness, existence, and stability, as well as a priori error estimates for the spatial and temporal errors are established. A space-time non-overlapping domain decomposition method is developed that reduces the global problem to a space-time coarse-scale mortar interface problem. Each interface iteration involves solving in parallel space-time subdomain problems. The spectral properties of the interface operator and the convergence of the interface iteration are analyzed. The method is implemented in a code based on the deal.ii parallel library. We illustrate the behavior of the method on several examples that highlight the advantages of the multiscale mortar space-time domain decomposition method.

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MS48

Unsaturated Flow in the Presence of Fractures Acting As Capillary Barriers

In this talk, I will present a model for unsaturated flow in fractured porous media. The model uses Richards' equation to describe the flow in the soil. However, unlike standard models that use a cubic-type law inside the fractures, we assume that water can enter into the fractures only if the capillary barrier is overcome. Once water entered into a fracture, we assume that it is in hydrostatic equilibrium. The resulting set of equations can then be classified as a coupled non-linear PDE-ODE system with variational inequalities. Solving numerically such type of systems is non-trivial due to the large pressure gradients and the presence of the capillary barriers. In this talk, I will explore three linearization methods to solve the discretised problem: e.g., Newton method, modified Picard iteration, and the L-scheme; and I will show a comparison of their performance.

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MS48

Mixed Finite Elements for Thermo-Hydro-Mechanical Models with Iterative Coupling

In this talk, we discuss a sequential computational scheme for the thermo-hydro-mechanical coupling in ice-rich porous media such as permafrost. The model describes energy conservation of freezing/thawing processes coupled to Biots poroelasticity system. For spatial discretization of the thermal model, we employ a fully implicit P0-P0 algorithm for the (temperature-enthalpy) pair based on the lowest order mixed finite elements: we demonstrate the robustness and convergence of the approach and some special nonlinear solver techniques necessary in domains with heterogeneous structure. Next we present the features of the three field Q1-P0-RT0 approach for the hydro-mechanical (Biot) model with focus on the new challenges when the freezing/thawing processes predicted by the thermal model change the flow and elastic properties of the domain. Finally we discuss the robustness of the entire iterative procedure.

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MS49

Arbitrary Order Discontinuous Galerkin Method in Time and Space with Lagrange Multiplier for NonlinearHyperbolic Conservation Laws

Arbitrary order discontinuous Galerkin method in time and space with Lagrange multiplier is proposed to approximate the solution to nonlinear hyperbolic conservation laws with boundary conditions. Stability of the approximate solution is proved in a broken $L^2(L^2)$ norm and also in an $l^\infty(L^2)$ norm. Error estimates of $\mathcal{O}(h^{r+\frac{1}{2}} + k_n^{q+\frac{1}{2}})$ with $P_r(E)$ and $P_q(J_n)$ elements $(r, q \geq \frac{d+1}{2})$ are derived in a broken $L^2(L^2)$ norm, where h and k_n are the maximum diameters of the elements and the time step of J_n, respectively, J_n is the time interval, and d is the dimension of the spatial domain. An explanation on algorithmic aspects is given. P_0 time and space subcell limiting processes are applied to resolve the shocks. Some numerical examples for advection, shallow water, and compressible Euler equations are presented.

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MS49

Staggered Dg Methods for Darcy-Forchheimer Flows on General Meshes

In this talk, we present a staggered discontinuous Galerkin method for the Stokes and Darcy–Forchheimer problems coupled with the Beavers–Joseph–Saffman conditions. The method is defined by imposing staggered continuity for all the variables involved and the interface conditions are enforced by switching the roles of the variables met on the interface, which eliminate the hassle of introducing additional variables. This method can be flexibly applied to rough grids such as the highly distorted grids and the polygonal grids. In addition, the method allows nonmatching grids on the interface thanks to the special inclusion of the interface conditions, which is highly appreciated from a practical point of view. A new discrete trace inequality and a generalized Poincar–Friedrichs inequality are proved, which enables us to prove the optimal convergence estimates under reasonable regularity assumptions. Finally, several numerical experiments are given to illustrate the performances of the proposed method, and the numerical results indicate that the proposed method is accurate and efficient, and in addition, it is a good candidate for practical applications.

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MS49

Physics-Preserving Enriched Galerkin Method for Thermo-Poroelasticity

In this talk, we are concerned with a numerical modeling framework for thermal-hydraulic-mechanical (THM) processes described by Biots thermo-poroelasticity model. We propose a coupled enriched Galerkin (EG) method utilizing two types of EG methods to provide a robust and physics-preserving method for the governing model. The proposed EG scheme is mass and energy conservative and free of numerical instabilities, commonly present in poroelasticity and coupled flow-transport problems. We will present theoretical aspects of mass and energy conservation properties and optimal convergence of the proposed EG method. We will also provide some numerical examples to confirm the results of our theoretical study.

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MS49

A Strongly Mass Conservative Scheme for Coupled Flow and Transport

In this talk, I will present a viscosity robust scheme for solving coupled Brinkman-Darcy flow and transport. The staggered DG method and mixed finite element method are judiciously combined to yield a strongly conservative scheme, which is particularly important for practical applications. Moreover, the interface conditions are enforced without resorting to Lagrange multiplier, and the continuity of the normal velocity is also satisfied at the discrete level. The optimal convergence error estimates of the scheme for all the involved variables are rigorously proved. Several numerical experiments will be presented to verify the performance of the proposed scheme.

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MS50

In-Situ Inference: Bringing Advanced Data Science into Exascale Climate Simulations

The unprecedented complexity of data generated by exascale simulations will open up new avenues of scientific discovery. But it is not generally feasible to save out all the data, due to storage limitations. The missing science is the ability to fit or train complex statistical models (statistical inference) as the simulations are running. Barriers to in-situ inference include the ability to statistically model spatiotemporal data in a scalable, distributed, ”streaming” setting (where data at previous times is overwritten), as well as high-level programming abstractions for data scientists to productively write general, portable, and performant analysis code. During this talk, I will discuss a number of advances in statistical inference and in-situ computer science which include sparse gaussian processes, distributed PCA and feature-driven methods based on topology and Gaussian mixture models. They serve as the building blocks for a very general class of inference problems, the hierarchical Bayesian spatiotemporal model. Machine learning is used to accelerate inference by learning data features to minimize distributed data communication. Our implemented in-situ programming environment significantly improves data science productivity, allowing data scientists to write powerful, concise, parallelized statistical algorithms with higher-level programming abstractions than Fortran/C++ and MPI.

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MS50

Fusion of a Machine Learning and Climate Model to Embed High Resolution Variability into a Coarse Resolution Climate Simulation

High resolution global climate simulations are computationally intractable due to the integration over long time scales. Therefore coarse spatial resolution models are used. One of the known failings of current climate simulations is the underrepresentation of cloud formation, which is largely due to the disparity in the spatial scale of the model and the underlying cloud generating physical processes. In this work emphasis has been placed on fusing ML techniques with a climate model so as to embed high resolution variability into a coarse resolution climate model - with the aim of improving the representation of convective cloud formation. A multi-output Gaussian Process (MOGP) is trained on high resolution Unified Model (UM) runs to predict the variability on the temperature and specific humidity fields. A proof of concept study has been carried out where the trained MOGP model is then coupled in-situ with a simplified Atmospheric General Circulation Model (AGCM) named SPEEDY. The mean profiles of the SPEEDY model are perturbed at each timestep according to the predicted high resolution informed variability. The climate statistics from the fused ML and SPEEDY model are then compared to the pure model run. Improvements in the precipitation, outgoing longwave and shortwave radiation patterns are observed.

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MS50

A Hybrid Approach to Earth System Modeling

This talk describes a hybrid modeling approach that combines machine learning (ML) with a physics-based numerical model of one or more components of the earth system. The potential of the hybrid approach is demonstrated with an implementation on a low-resolution simplified-physics atmospheric global circulation model (AGCM). It is shown that the hybrid model provides more accurate forecasts and has a more realistic climate than the AGCM. The hybrid model can even capture dynamical processes not captured by the AGCM. For the AGCM of the present talk, one such process is sudden stratospheric warming (SSW). The approach also provides a flexible framework to introduce additional (ML-based) prognostic model variables. It is shown that introducing 6-hour cumulative precipitation and sea surface temperature (SST) as additional prognostic variables leads to a realistic precipitation climatology and ENSO signal in the SST and atmospheric surface pressure.

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MS50

Uncertainty Quantification for Running Individual Climate Models in Coupled Mode, with Application to Coupled Climate and Ice Sheet Simulations of the Last Glacial Maximum

Climate models are really lots of models coupled together. To a climate modeller, the ”coupled model” is usually the atmosphere and ocean coupled together and must be run sparingly, because it is much much slower to evaluate (and requires more spinning up) than, say the atmosphere only model. This type of explicit coupling is common when big processes are modelled independently (e.g. ice sheets, aerosols, carbon cycles), but we might also think of the atmosphere as a series of coupled processes (radiation, convection, ...). The drive to run coupled so that feedbacks are felt or proper boundary condition uncertainty captured, is strong, and yet coupling can completely eliminate the possibility for uncertainty quantification through increasing computation time by orders of magnitude. This talk will discuss using UQ to make the model ”feel” the coupled model without coupling directly. We have 2 examples, one when running a coupled ice-sheet atmosphere over Palaeotime scales requires an dynamic ocean boundary condition that is consistent with sparse observations, and another where a fast ice sheet model receives its boundary conditions from an atmosphere model during the simulation.

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MS51

Uncertainty Quantification and Data Fusion for Remote Sensing Data

Remote sensing data produced by NASA and other space agencies are a vast resource for the study of Earth's system, and physical processes which drive it. However, no remote sensing instrument actually observes these processes directly; instruments collect electromagnetic spectra aggregated over two-dimensional ground footprints or three-dimensional voxels. Inference on physical state occurs via complex ground data processing operations featuring retrieval algorithms, so named because they retrieve latent true states from spectra. Data Fusion is defined here as joint inference about true states using multiple retrieved data sets as inputs. The inputs have different sampling characteristics, including uncertainties and geometries. Fusion is worthwhile if it can capitalize on complementary strengths of the inputs including spatial and temporal data structure. Optimal fusion estimates can be made if 1) uncertainties on the inputs are provided, and 2) a statistical model that accounts for heterogeneities, and properly handles spatial and temporal change-of-support, is used. This talk will introduced formalisms for both Uncertainty Quantification and Data Fusion in the context of remote sensing, and will discuss how we at JPL implement them in a practical way that demands we keep up with data flow. Examples will be drawn from experiences in Uncertainty Quantification and Data Fusion for a number of different current and future NASA missions.

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MS51

Data Fusion with Uncertainty Quantification for Observational Data

Observational data for earth system monitoring is available in abundance, but it is often incomplete due to inconsistent collection. Combining information from disparate sources can create more complete datasets but if done haphazardly, can lead to misleading conclusions. Existing combined data products often do not provide uncertainty quantification nor near-real time data streams, and although there are many proposed data fusion techniques, many are not readily implementable. In this talk, we will present a methodology that is straightforward to implement, transparent, and is generalizable for many variables of interest. It accounts for non-stationarity as well as the change of support problem that makes uncertainty quantification difficult for areal (spatially-aggregated) datasets. We demonstrate using three atmospheric variables: temperature, aerosol optical depth, and net radiative flux and show we can produce a complete dataset, at a flexible range of resolutions, that accounts for spatial and temporal autocorrelation. Computing time scales with the computational resources available to the user. Fused datasets can support a variety of statistical and machine learning models, and because they include uncertainty quantification, they can be used for improving validation efforts of climate models and re-analysis data products.

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MS51

Hierarchical and Partitioned Sparse Variational Gaussian Processes for In-Situ Inference

The next generation of Department of Energy supercomputers will be capable of exascale computation. For these machines, far more computation will be possible than that which can be saved to disk. 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. In this talk, we discuss several recent methodologies which arise as extensions of sparse variational Gaussian processes and we demonstrate the effectiveness of the methods for simulations from the Energy Exascale Earth System model (E3SM).

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MS52

Simulation of Thermo-Poroelasticity Using Enriched Galerkin and a Modified Method of Characteristics

We present the mathematical formulation of discretizing thermo-poroelasticity problems by the method of characteristics for the energy balance equation, Enriched-Galerkin for fluid flow, and continuous Galerkin for mechanics. Because of the low thermal conductivities in rocks, the thermal response is dominated by the convection of the fluid flow. Thus, the temperature field has a nonlinear heterogeneity with a sharp-moving front in the case of an injection-production geothermal system. Simulating the energy balance utilizing conventional continuous Galerkin (CG) suffers from grid orientation and numerical dispersion problems and embeds the ability to progress the simulation with large time steps. Therefore, we utilize a modified method of characteristics to model the energy balance PDE that enables large time-stepping without a loss in the simulation accuracy. It also minimizes the overshooting difficulties at the sharp interfaces compared to the CG discretization scheme. The mass balance PDE is solved with the Enriched Galerkin (EG) scheme to ensure the local mass conservation of the pressure field with minimal computational cost. The EG scheme is developed by enriching the CG scheme with piecewise discontinuous constants. Numerical results on a variety of analytical and experimental thermo-poroelasticity problems show matching results, reduced effects of numerical dispersion, and front overshoot, along with minimal energy and mass balance errors.

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MS52

Multiphysics Phase-Field Modeling and Efficient Numerical Solution in Fractured Porous Media

In this presentation, we explain our computational IPACS (Integrated Phase-field Advanced Crack Propagation Simulator) framework for solving multiphysics phase-field fracture problems in porous media. Therein, the following five coupled nonlinear physical models are addressed: displacements (geo-mechanics), a phase-field variable to indicate the fracture position, a pressure equation (to describe flow), a proppant concentration equation, and/or a saturation equation for two-phase fracture flow, and finally a finite element crack width problem. The overall coupled problem is solved with a staggered solution approach, known in subsurface modeling as the fixed-stress iteration. A main focus is on physics-based discretizations. Galerkin finite elements are employed for the displacement-phase-field system and the crack width problem. Enriched Galerkin formulations are used for the pressure equation. Further enrichments using entropy-vanishing viscosity are employed for the proppant and/or saturation equations. A robust and efficient quasi monolithic semi-smooth Newton solver, local mesh adaptivity, and parallel implementations allow for competitive timings in terms of the computational cost. Our framework can treat two- and three-dimensional realistic field and laboratory examples. Representative numerical examples are illustrate the capabilities. IPACS is built upon the finite element library deal.II.

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MS52

Scaled Capillary Pressure and Its Hysteresis with Gas Production from the Gas Hydrate Deposit

We investigate the hysteresis phenomena with the scaled capillary pressure in the gas hydrate deposit. For the scaled capillary pressure, the permeability scaling factor is applied to capillary pressure as Leverett's model based on the porosity and permeability change. Upon the scaled model, non-monotonic capillary pressure can be observed due to the increased gas saturation and decreased hydrate saturation when hydrate dissociation occurs. For its hysteretic behavior, we employ the authors' previously proposed numerical approach for the hysteretic capillary pressure and relative permeability, which is based on the 1D elastoplasticity algorithmic framework. This approach yields contractivity and algorithmic stability for the hysteretic behavior between capillary pressure and water or aqueous phase saturation. The scaled capillary pressure and its hysteresis are coupled with the geomechanics through the fixed-stress sequential method for its two-way coupling. In the numerical experiments for natural gas production in a reservoir through depressurization, we compare 4 cases for the capillary pressure model: the non-scaled-only (basic), non-scaled-with-hysteresis, scaled-only, and scaled-with-hysteresis. The results indicate that although the scaled capillary pressure can bring the poromechanical effects enhancing the geomechanical stability, further stimulation strategy such as hydraulic fracturing is necessary when hysteresis is considered simultaneously.

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MS52

Poro-Elastic Coupling with Diffused Fracture in Phase-Field Models

Since their inception in late 90's, the phase-field models of fracture simulation have become one of the standard numerical approaches. One of the appeals is their ability to handle initiation and propagation of any number of fractures with an arbitrary geometry in a unified manner. And it has been extended to hydraulic fracturing by incorporating the hydraulic force in fracture as external work in the variational formalism. Although various formulations of phase-field hydraulic fracturing have been proposed to date, some details yet remain to be established such as fracture aperture, fluid leak-off, or delineation of the fractures in their diffused representations of fractures. In this study, we explore previously proposed models with diffused fractures and assess their accuracy in terms of their ability to recover the explicit fracture properties such as fracture aperture or critical energy. We then propose a poro-elastic energy function with diffused fractures and diffused poro-elastic properties and compare the responses against closed form solutions. Finally, we demonstrate the models ability to handle versatile problems with illustrative examples relevant to geoscientific applications.

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MS53

Design and Validation of a Shallow Water Model for Meteo-Tsunami Simulations

Meteo-tsunamis are wave phenomena similar to earthquake-induced tsunamis occurring in shallow seas. The amplitudes may be in the meter range and runup heights may reach several meters, posing a threat to coastal communities. The main source mechanism triggering such waves is a resonance of a meteorological disturbance, such as a local front or low pressure area, with the gravity wave speed of the water column. Such a phenomenon can well be represented by a shallow water type model, with atmospheric pressure and wind forcing terms added as external forcing to the equations. In this presentation, we will introduce a shallow water simulation code, based on a Runge-Kutta Discontinouous Galerkin (RKDG) discretization with adaptive mesh refinement. Our code base has been successfully used for tsunami simulations and was validated by well-accepted test cases. The code was then extended for the application to meteo-tsunamis and a new set of test cases for this type of applications was compiled. We show results of our simulations to the meteo-tsunami test suite and evaluate the efficiency of adaptive mesh refinement for such applications.

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MS53

Development of a Digital-Twin for Probabilistic Tsunami Forecasting

A new Digital Twin (DT) for Probabilistic Tsunami Forecasting (PTF) presently under development is presented here. The first version of this DT is a PTF that combine early estimation of earthquake parameters with large ensembles of urgent shallow water tsunami propagation simulations using the Tsunami-HySEA model (Selva et al. 2021, Nature Commun.). In this first PTF, earthquake information is conveyed to the tsunami model only during forecasting initiation. For the new Digital Twin, continuous data assimilation for an extended set of data sources (e.g. improved earthquake solutions, sea level tsunami data, GNSS) will enable a close to real time synthesis of data products and modelling, updating the model based on the incident data stream. In addition, the DT will be modularised to allow for including improved wave and source physics through dispersion, non-hydrostatic generation, inundation improved earthquake physics, and cascading earthquake triggered landslide tsunamis. In the presentation we will present the first version of the PTF, followed by an outline of the design of the new digital twin, as well as briefly describing the present status and plans for further development. This work is supported by the European Unions Horizon Europe Research and Innovation Program under grant agreement No 101058129 (DT-GEO, https://dtgeo.eu/).

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MS53

Unique Insight into Landslide Dynamics from Inversion of Seismic Data Combined with Numerical Modelling of the Processes

Landslides represent one of the costliest geo-hazards and a growing threat to human life across the globe as a result of climate change and population growth. Although landslides are hard to observe directly, their signature is available in the form of the seismic waves that they generate. Interpretation of these waves in terms of physical processes is a challenge that can only be addressed through state-of-the-art numerical modelling of landslides as will be shown here. Indeed, the complex effects of topography, rheology, initial released mass, etc. are all mixed up in the generated seismic signal. However, comparing the force inverted from low frequency seismic data with a series of landslide simulations makes it possible to recover the shape and volume of the initial mass, the rheological parameters, as well as other processes such as the presence of a glacier on the landslide trajectory or erosion effects. Going further in this direction requires improving landslide models to get insight into the unexplained high mobility of large landslides.

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MS53

Towards Fully Physics-Based Seismic and Tsunami Hazard Assessment

Seismic and tsunami probabilistic hazard assessment and early warning systems typically rely on kinematic orstochastic earthquake models. Self-consistent 3D simulations of dynamic earthquake rupture with linked or fully coupled tsunami (Krenz et al., SC21, Abrahams et al., preprint, Eartharxiv, 2022) can provide building blocks towards fully physics-based hazard analysis. We here show how tectonic, geologic, geodetic and seismic observations can be used to constrain suites of plausible Hellenic Arc subduction and highly segmented Northern Iceland strikeslip earthquake and resulting tsunami scenarios (Bo Li et al., preprint, Essoar, 2022) utilizing high-performance computing. Our models cannot only capture important aspects of dynamic earthquake-tsunami interaction but also shed light on fault system interactions, the associated seismic ground motions and maximum expected earthquake magnitude.

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MS54

Quadrature-Free Discontinuous Galerkin Method for Shallow Water Equations on Block-Structured Grids

In this talk, we address several techniques aiming to significantly improve the computational performance of numerical models of ocean as exemplified by our discontinuous Galerkin solver for shallow water equations on unstructured meshes. In particular, we re-formulate the system in such a way that allows to discretize it using a quadrature-free scheme. To allow code optimizations associated with structured-grid models we developed an block-structured grid generator for complex ocean domains.

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MS54

Psyclone - a Weather and Climate Code-Transformation System

PSyclone is a code-generation and transformation system designed to assist Fortran weather and climate models to achieve performance portability while keeping maintainable single-source software codebases. It does this by creating an Intermediate Representation of the code that can be extended with application domain-specific concepts and can be manipulated by HPC performance experts through PSyclone scripts. PSyclone is used in the LFRic Project, the next generation atmospheric model of the UK Met Office, to support its domain-specific language (DSL) and produce distributed and shared memory parallel implementations of the model. It is also used with different configurations of the NEMO model, where PSyclone is able to process an unmodified version of the base software and automatically insert threading and GPU offloading capabilities to improve the performance of the application on modern heterogeneous systems. It is planned to be integrated as an optional component of the NEMO build system.

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MS54

Experience with Parallel-in-Time Algorithms for Academic and Operational Climate Models

The availability of high numbers of processors in HPC systems gave rise to ideas for parallelization beyond the classical domain decomposition approach. Lions Maday Turinici introduced the so-called Parareal algorithm in 2001. In this method, a pair of coarse (fast) and fine (slow) time integrators is used. The original fine solver is applied on time slices in parallel, and coarse correction runs are used to obtain convergence. It turns out that the algorithm converges well for diffusion-dominated problems, but has problems for advection-dominated ones. There are ideas to overcome this difficulty. In this talk, we show successful applications of the method in academic cases. When it comes to real-world or operational climate models, technical problems of software and data handling dominate the pure mathematical convergence issues. As example, we show our work with the ocean model FESOM2.

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MS55

Differential Complexes for Modelling in Porous Media

We consider a hierarchy of domains structured such that each lower-dimensional domain is contained in the boundary of a domain that is of one dimension higher. Partial differential equations on such structures are called mixed-dimensional problems, and they are used in modelling of fractured porous media. The function spaces considered in mixed-dimensional problems together with their associated linear differential operators form what is called a cochain complex; a sequence of vector spaces where successive use of two such differential operators yields zero. Another example of a cochain complex is the Cech-de Rham complex. It is obtained by considering a geometry of overlapping domains rather than domains which shares common boundaries. The purpose of the talk is to introduce the mixed-dimensional de Rham complex and the Cech-de Rham complex, discuss how they can model fractured porous media and show the relationship between the two complexes.

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MS55

Network Models for Pulsatile Perivascular Fluid Flow

Alzheimers disease is characterized by the accumulation of toxic proteins in the brain. The initiation of the disease is poorly understood, in part because it is not known what physical processes are actually responsible for clearing these proteins. According to the glymphatic theory, waste removal is facilitated by a bulk flow of CSF through a network of perivascular spaces surrounding the vasculature of the brain. The validity of this hypothesis is currently being scrutinized using e.g. numerical simulations. In this talk, we present a 1D Brinkman-Stokes type network model for perivascular fluid flow. We show how the network model can be discretized using finite elements and connect the properties of the discretization to the properties of the network graph. The network model accounts for fluid flow driven by both pressure gradients and arterial pulsations. We show how the numerical simulations connect to fundamental questions regarding the glymphatic theory; in particular, we show that traveling vasomotion waves are capable of driving net fluid flow through the network.

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MS55

1D-3D Coupling Concepts for Thin Embedded Networks in the Context of Richards Equation

Porous media with *embedded transport network systems* are found in various applications, for example, heat exchangers, geothermal wells, or root water uptake. When the network is embedded in the *unsaturated soil zone*, the Richards equation provides a simplified description of two-phase flow in the soil domain. Due to the nonlinear dependence of the hydraulic conductivity on the soil water saturation, large local pressure gradients can occur when water is being extracted from the soil, for example, by roots. When designing mathematical models and numerical methods to simulate such systems, we face two major issues: (1) The embedded network elements are *thin*. (2) The solution is *highly nonlinear* and can exhibit singularities in the vicinity of the network. The second problem is largely amplified for the Richards equation in comparison to linear single-phase flow equations. For root water uptake, we demonstrate that models typically used today, fall short of solving the proposed model equations accurately. We present results from a recent benchmark study and a test case exposing current issues. We then present in detail an *explicit-* and an *implicit-interface method* to solve root-water uptake problems formulated in terms of embedded networks and soil models based on Richards equations accurately. Comparisons of the schemes are shown for both *steady-state* and *transient* simulations.

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MS55

Advection-Reaction Simulations with Growing 1D Networks in Porous Domains

Simulations in domains with embedded tubular inclusions with radius much smaller than characteristic length are still challenging. Indeed, the generation of a computational mesh capable of resolving inclusion size might result in linear systems with a very large number of unknowns. Further, for complex networks of inclusions, the whole mesh generation process might result unfeasible, due to the large number of constraints. The situation is even more complex in time-dependent simulations where inclusions are allowed to change with time. The geometrical reduction of the inclusions to 1D objects can mitigate the computational cost and allows the treatment of arbitrarily complex configurations. The 3D inclusions are collapsed on their centrelines, and, simultaneously, the external domain is extended to fill the voids. The resulting problem becomes a 3D-1D coupled problem. Here a domain decomposition approach for this kind of coupling is presented and applied to realistic simulations with growing 1D networks in a bulk 3D domain. The method is based on a PDE constrained optimization approach allowing the use of non-conforming meshes at the interfaces.

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MS56

The Impact of Fluid Pressure and Rock-Matrix Volume Strain of Fracture Aperture in Fractured Rock Masses

Fracture aperture has a decisive influence on the outcome of discrete fracture and rock matrix (DFM) fluid flow simulations but varies among fractures and along their planes. It is a dynamic parameter dependent on fluid pressure and ambient stress and is difficult to observe under in situ conditions. Focusing on partially sealed fractures in carbonates, a range of studies have determined systematic relationships between fracture length and maximum aperture. However, attempts to invert the length-over-width ratio of vein fills of such fractures for the in situ stress while assuming a linear elastic rock matrix, yield implausibly high stress values. A potential explanation of these small aspect ratios is that the rock matrix actively contracted during fracture growth. Such shrinkage is a well-documented process accompanying compaction, diagenesis, and dewatering of sediments during burial. Here we use DFM models built from trace maps of layer-restricted syn-diagenetic fractures to investigate matrix-contraction-assisted fracture opening using the finite-element method. Modelling fractures as detached boundaries with intervening lower-dimensional surfaces, aperture distributions obtained by pressure inflation are contrasted with ones obtained by matrix shrinkage. The best fits are selected by comparison with apertures preserved in the field data. Additional modelling considers viscous stress dissipation as a further mechanism to explain the stubby veins.

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MS56

Use of Gradient and Ensemble Based Data Assimilation Methods for Quantifying Reservoir Geomechanics Uncertainties

In this work, we explore the use of gradient and ensemble based data assimilation methods for quantifying uncertainties in geomechanical responses of reservoirs in energy transition applications. By combining a physics-based proxy formulation for geomechanics with the Delft Advanced Research Terra Simulator (DARTS), we are able to compute sequentially the geomechanical responses of the reservoir development, including stress and displacement as well as flow responses. We apply both the Ensemble Smoother with multiple Data Assimilation (ES-MDA) and Randomized Maximum Likelyhood (RML) methods to quantify uncertainties in geomechanics parameters. Through case studies, we evaluate the proposed workflow and demonstrate its effectiveness in quantifying uncertainties when geomechanics is taken into account. We also discuss the potential benefits and limitations of these methods for reservoir management and development, highlighting their potential to inform more accurate predictions of reservoir behavior. Additionally, our study provides valuable insights into the role of data assimilation in improving our understanding of the subsurface and supporting effective decision-making in the energy industry.

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MS56

Fast and Accurate Estimation of Evapotranspiration Rates from Distributed Moisture Sensors

Smart agriculture and sustainable groundwater management require the ability to quantify evapotranspiration (ET). Efficient ET estimation strategies often rely on the vertical (one-dimensional) flow assumption to assimilate data collacted by soil moisture sensors. While adequate in some applications, this assumption fails when horizontal flow is not negligible due to, e.g., soil heterogeneity or drip irrigation. We present two novel implementations of the ensemble Kalman filter (EnKF) that uses the ET sink term in the Richards equation as the updatable observable and maximum likelihood estimator (MLE) to infer spatially varying evapotranspiration rates and root water uptake profiles. We test the prediction accuracy and computational efficiency of our methods in a setting representative of drip irrigation. Our strategies outperform the standard EnKF approach that uses soil moisture as the updatable variable: they accurately estimate the total ET rates and root profiles up to two orders of magnitude faster than the standard EnKF.

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MS56

Using ES-MDA to Improve Field Geomechanical Management

A geomechanical model is a valuable tool that improves the development plan of oil and gas fields. It brings insights into the crust stress state, preferential flow direction, potential reservoir compaction, expected subsidence, the associated hydraulic impairment, and geohazard risks. Given the general irreversible nature of these phenomena, the anticipation of their onset and severity is key to a successful reservoir management strategy. However, information on the rock poromechanical behavior is scarce, especially outside the reservoir strata and in the initial stages of the field appraisal phase. In this context, it is desirable to work with multiple scenarios. Recent advances in Petrobras in-house finite element simulator (GeomecBR) have significantly reduced the time required to run a geomechanical analysis, allowing the incorporation of uncertainty assessment in the workflow. In this study, we propose a probabilistic workflow using the ES-MDA method to estimate uncertainties in input parameters while assimilating stress measurement data. We apply it to a pre-salt field operated by Petrobras, showing that it accurately preserves stress field variability while honoring the stress measurements. The visualization of regions of high uncertainty in SKUA-GOCAD aids in confident decision-making for field management and data acquisition planning.

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MS57

Feature Importance with Deep Echo State Models

Climate change due to human activity is considered a serious threat to our future. Climate intervention methods, such as solar radiation management, to reduce the negative impacts of climate change are becoming a real possibility. The development of algorithmic methods for understanding the short-term and long-term impacts of such events on climate change will help inform decision makers. Deep ensemble echo-state network (D-EESN) models may provide a route to assist with modeling the dynamic climate impacts. D-EESN models offer increased computational efficiency over other statistical spatio-temporal methods and provide uncertainty quantification through bootstrapping. However, D-EESN models are currently only able to provide forecasts and lack general interpretability. We are interested in developing methodology for understanding the relationships between the D-EESN inputs and outputs to help identify early indicators of significant climate impacts. We propose a variable importance technique for D-EESNs that returns the temporal importance of an input variable on forecasts. We demonstrate our methodology on reanalysis data that includes the 1991 eruption of Mount Pinatubo. We forecast stratospheric temperature given lagged stratospheric temperature and aerosol optical depth, and we use the proposed variable importance to capture the relationships between variables and how those relationships change over time.

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MS57

Sequential Conformity Testing with Black Box Counterfactuals

We propose a new policy evaluation procedure for multivariate and functional processes based on counterfactual prediction and a sequential version of conformal p-values. We view causal effect detection as a sequential outlier detection problem where we sequentially test if post-intervention samples belong to the pre-intervention distribution until we detect a change and declare the intervention effective. In our approach, any black box model can be used to forecast a counterfactual process in absence of the intervention and our sequential conformity test will provide marginally valid p-values for distributional change detection. We show that our method, like other conformal methods, is finite sample valid and powerful under many alternatives regardless of the underlying predictive model or outlier detector. We demonstrate our method's empirical finite sample performance and apply it to volcanic eruption data to detect distributional changes in spatially-varying temperature profiles.

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MS58

Hybridizable Discontinuous Galerkin Methods for Coupled Systems of Poroelasticity and Free Flow Equations

In this work we develop and analyze hybridizable discontinuous Galerkin (HDG) methods for problems such that the Stokes and Navier-Stokes equations and the Biot consolidation equations are coupled with interface. In our HDG methods the compressibilities of fluid and poroelastic matrix, and the fluid mass in poroelastic domain are strongly conservative. This is a joint work with Aycil Cesmelioglu at Oakland University and Sander Rhebergen at University of Waterloo.

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MS58

Numerical Modelling of Coupled Thermo-Hydro-Mechanical Multiple Fracture Growth in Three Dimensions

Multiple fractures are grown in a three-dimensional volumetric domain subjected to thermal loads. Coupled partial differential equations for thermo-poro-elastic deformation are solved using the finite element method. The matrix is assumed to be linear elastic and isotropic, Darcy flow is assumed in the matrix and laminar flow is assumed in the fractures. The volume is discretised by tetrahedral and hexahedral meshes, using isogeometric quadratic elements. Fractures nucleate in response to the local accumulation of damage. Fracture geometry is represented by NURBS surfaces, which are discretised using quadrilaterals. Quarter point elements discretise the vicinity of the fracture tips. The virtual disk integration method is implemented to compute modal stress intensity factors. Growth angles are computed using the Richard method, resulting in propagation vectors that modify the discrete geometry of the resulting non-planar fractures. After each growth event the mesh is regenerated and optimised to the new geometry. Fractures grow and interact in response to thermal loads, and their geometries are modified accordingly. Examples of growth are shown in the context of fracturing around deposition boreholes for nuclear waste storage, and the thermal shock of a ceramic plate. Resulting patterns are compared against experimental and field observations.

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MS58

From Pore to Darcy Scale in Permafrost

Permafrost is "frozen ground' abundantly featured in the Arctic, and its thermal state is closely linked to the global climate controls. In the talk we present our recent results on upscaling realistic physical model of thawing and freezing at the pore-scale to the permafrost scale. The pore-scale model is a heterogeneous Stefan problem which accounts for (i) different thermal properties of the mineral and water phases as well as for (ii) additional physical effects due to thermodynamics in confined regions. The challenges include computational difficulties in (i) related to the discontinuities at material interfaces, as well as modeling challenges for (ii) which we link to Gibbs-Thompson law. The pore-scale model is next upscaled to Darcy scale at which it is compared to the constitutive properties of ice-rich soil found empirically, with good agreement. We next compare the solutions to both models. We also consider upscaling of properties of flow from pore-scale to Darcy which must account for thin water film around the grains; this prevents the permeability from going to zero as the ice phase forms.

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MS58

Modeling and Simulation of Fracture Deformation in Coupled Problems

In tight rocks, fractures provide a large part of the potential for fluid flow. However, the fractures are closed with minute hydraulic aperture under many typical subsurface conditions. This has led to high interest in permeability engineering through induced aperture enhancement. In this talk, we study three modes of stimulation: normal opening with mechanical separation of the fracture walls, elastic normal deformation with mechanical contact and shear stimulation. Similarly, we distinguish between two driving mechanisms for stimulation: pressure enhancement and cooling induced rock contraction. Significant effort has been made to study pressure driven stimulation. Thermal reduction is less studied, despite being identified as contributing significant to overall aperture increase in applications involving cold injection fluid. We study the interplay between the two driving forces and the three modes through numerical simulations using the PorePy simulation toolbox. The 3d simulation scenarios are designed to mimic relevant reservoir conditions with circulation of cold fluids.

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MS59

A Parameter-Free Adaptivity Indicator for a P-Adaptive Discontinuous Galerkin Discretization of the Shallow Water Equations

We propose a parameter-free adaptivity indicator for a p-adaptive quadrature-free discontinuous Galerkin discretization of the shallow water equations. It aims to identify resolved and under-resolved solution parts while distinguishing between smooth and non-smooth regions without utilizing any problem-dependent parameters. The information collected for slope limiting is used to detect the error and smoothness of the solution. For piecewise constant discretizations, the indicator first performs a reconstruction procedure. The accuracy and robustness of the new scheme are evaluated using several benchmarks from the literature and compared to other adaptivity indicators. Our results indicate that the proposed indicator finds a good balance between solution quality and computational overhead.

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MS59

MCMC Methods for Shallow Water Source Inversion

UM-Bridge is an easy to use and language-agnostic software interface for coupling Uncertainty Quantification (UQ) methods to numerical models. It enables containerization of models for portability and reproducibility as well as access to cloud platforms. Using the UM-Bridge interface we have we modeled the propagation of the 2011 Tohoku tsunami by solving the shallow water equations. For the numerical solution of the PDE, we apply an ADER-DG method implemented in the ExaHyPE framework. The aim is to obtain the parameters describing the initial displacements from the data of two available buoys located near the Japanese coast. To do so we have applied a novel multilevel Markov Chain Monte-Carlo (MLMCMC) method. In this talk I will discuss both how to use the generic UM-Bridge interface in order to easily apply state-of-the-art UQ methods to complex forward models, as well as the tsunami source inversion itself.

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MS59

Implementing High-Order ADER-DG to Model Shallow Water Waves with Dispersion in sam(oa)

sam(oa) is a parallel adaptive mesh refinement package for solving 2D PDEs on dynamically adaptive triangular meshes. It comes with various solvers for the shallow water equations, including a high-oder discontiunous Galerkin scheme with ADER time stepping. We will report on recent work to extent this solver towards models that consider dispersion - considering both aspects of accuracy of the DG scheme, and achieved parallel performance.

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MS59

2D Shallow Moment Equations for Geophysical Applications

Shallow water models are successfully used for simulating geophysical flows like river floods, tsunamis, sediment transport, or debris flows. While depth-averaged models are computationally very attractive, information on the vertical velocity is required a priori, typically by assuming a parametrized profile using a time-independent function, e.g. a constant. An extension of such models is introduced in the *shallow moment method*. This method retains transient information about the vertical flow profile by using a finite Legendre expansion to resolve said vertical velocity with time-dependent coefficients. The *shallow moment* approach allows to include more information systematically and generates a hierarchy of models that in the limit, recover the reference equations before depth-averaging and are therefore vertically fully resolved. However, even a low number of basis functions significantly increases the model's predictive power compared to classical shallow water systems. The *shallow moment method* has mostly been studied in a 1d setting assuming a Newtonian fluid. In the talk, we will summarize the fundamentals and discuss current developments involving the extension into two space dimensions, *dispersive shallow moment* systems that include non-hydrostatic pressure contributions and alternatives to a Newtonian closure in order to model more complex fluids, for example using the $\mu(I)$-rheology for granular flow problems.

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MS60

A Meeting of Stokes, Brinkman, and Darcy in Polytopal Multiscale Hybrid-Mixed Methods

H(div)-conforming velocity and discontinuous pressure approximations, usually applied for mixed Darcy's flow simulations, have been used by the authors in the design of innovative formulations of flow models in the whole Stokes-Brinkman range [hal-03867520,2022]. Hybridization is required for the weak enforcement of tangential continuity of the velocity by a properly chosen traction Lagrange multiplier. The method is strongly locally conservative and naturally gives exact divergence-free velocity fields. The current proposal is to evaluate a two-level version, denoted by MHM-H(div), guided by a well-posed characterization of the solution by components given by global-local systems subordinated to a flow domain partition by general polytopal subregions. The divergence-compatible finite element pairs for velocity-pressure used inside the subregions may be richer than the velocity normal trace and traction multiplier taken over their boundaries. Efficiency of computational implementation is achieved by the application of static condensation: the global system is solved for coarser variables composed by a pressure component piecewise constant over the polytopes, the velocity normal trace and the tangential traction over their interfaces. The refined components are recovered by solving independent local problems by the single-scale version of the method in each subdomain. Numerical results shall be presented for the verification of the main MHM-H(div) properties.

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MS60

Applications to Geosciences of Stabilization Free Virtual Element Methods

The aim of this talk is to present some application of a new family of Virtual Element Methods (VEM), designed to allow the definition of coercive bilinear forms that do not require an arbitrary stabilizing term. In many geophysical applications, the isotropic nature of the stabilization can introduce a non-physical perturbation of the model. Stabilization free VEM are developed in order to preserve the structure of the model problem, exploiting only polynomial projections in the discrete bilinear forms. The talk will focus on some interesting applications of the method, both in primal and in mixed formulation.

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MS60

A Fully-Discrete Virtual Element Approximation for the Time Dependent Boussinesq System

In this talk, we develop a fully-discrete virtual element discretization for the time dependent Boussinesq system formulated in terms of the stream-function and temperature fields. The discretization for the spatial variables is based on the coupling C^1- and C^0-conforming virtual element approaches, and we handle the time derivatives with a classical backward Euler implicit method. We provide the well-posedness and unconditional stability of the fully-discrete scheme. Furthermore, we derive error estimates in H^2- and H^1-norms for the stream-function and temperature variables, respectively. Finally, we present some numerical results to support the theoretical analysis and illustrate the behavior of the fully-discrete scheme.

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MS60

A Family of Virtual Elements for 3D Elasticity Problems

The Virtual Element Method is a recent numerical technology for the approximation of partial differential equations. In this talk, we present a family of Virtual Element Methods for three-dimensional linear elasticity problems. In particular, we consider the mixed formulation based on the Hellinger-Reissner functional. In this framework it is well known that, for classical Galerkin schemes, designing a suitable method that preserves both the symmetry of the stress tensor and the continuity of the tractions at the inter-element is typically not a simple task. The principal reason behind this difficulty lies in the rigid structure of the polynomial approximation space. Therefore, our idea is to exploit the great flexibility of the VEM to avoid these troubles and design stable methods. Finally, some numerical tests are provided in order to show the validity and the potential of our analysis.

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MS61

Rigorous Justification of Generalized Coupling Conditions for Stokes-Darcy Problems

Coupled free-flow and porous-medium flow systems occur often in nature as well as in a variety of technical applications. Pore-scale resolved simulations of such coupled systems are infeasible for practical purposes. Thus, alternative modeling approaches treating the fluid-porous system from a macroscale perspective are often applied. We consider the most widely studied model comprising the Stokes equations in the free-flow region and Darcy's law in the porous medium. The challenge is to formulate appropriate coupling conditions such that the Stokes-Darcy model reflects the pore-scale processes accurately. Since classical interface conditions are suitable for unidirectional flows only generalized coupling conditions are developed in [Eggenweiler & Rybak, Multiscale Model. Simul., 2021] via homogenization and boundary layer theory. These conditions are validated numerically by comparison of pore-scale and macroscale simulation results, however, justification of the underlying homogenization ansatz via rigorous error estimates is up to now an open question. In this talk, we extend the approximation of the pore-scale solution from [Eggenweiler & Rybak, Multiscale Model. Simul., 2021] by some higher order terms, derive modified generalized coupling conditions and prove rigorous error estimates for the new approximation. The importance of the additional higher order terms appearing in the new coupling conditions is analyzed for different flow regimes.

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MS61

Convergence Analysis of Discontinuous Galerkin Methods for Coupled Navier-Stokes and Darcy Problems

The coupling of free flow and porous media flow arises in several fields, such as energy, environment and biomedicine. This work focuses on the coupling of time-dependent incompressible Navier-Stokes equations with single phase flow. Interface conditions include the continuity of fluxes, the balance of forces and the Beavers-Joseph-Saffman condition. This talk reviews the error analysis of discontinuous Galerkin methods applied to both steady-state and time-dependent Navier-Stokes and Darcy equations. The effect of the interface conditions on the well-posedness of the problem is discussed. Key ingredients in deriving the a priori error bounds are presented.

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MS61

A Compact One-Domain Approach for Momentum Transport at Porous Media Boundaries

Momentum transport at porous media boundaries is usually modeled with a two-domain approach, which requires the use of coupling boundary conditions. While this approach has received significant attention over the past fifty years [1], a debate about the boundary conditions pertinence still lingering [2], a one-domain approach can also be considered. In this alternative, a single equation is used within the homogeneous portion of a porous medium and near the boundaries. Classically, a penalization procedure is used in which a Darcy-like term is added to the Navier-Stokes equations. Such equation is not of practical value due to its complexity and the difficulty to predict the spatial variations of the permeability. In this work, both limitations are surpassed by deriving a macroscale model that has a Darcy-like form and includes a closure scheme to predict the spatial changes of the permeability. The model is derived using a simplified volume-averaging method considering steady and single-phase flow under slip and inertial conditions. The model is validated by comparisons with pore-scale simulations [3] and also with experimental data showing excellent agreement [4]. References [1] Nield, D.A. (2009). Transport in Porous Media, 78, 537-540. [2] Eggenweiler E., Rybak I. (2020). Journal of Fluid Mechanics, 892, A10. [3] Valds-Parada F.J., Lasseux D. (2021). Physics of Fluids, 33, 073612. [4] Valds-Parada F.J., Lasseux D. (2021). Physics of Fluids, 33, 022106.

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MS61

An Augmented Fully-Mixed Formulation for the Navier-Stokes - Biot Model

We present a fully-mixed formulation and a mixed finite element method for the coupled problem arising in the interaction between a free fluid governed by the Navier–Stokes equations and a poroelastic medium modeled by the Biot system. We employ dual-mixed formulations in both domains and impose the transmission conditions weakly by introducing the traces of the structure velocity and the Darcy pressure on the interface as Lagrange multipliers. The fluid velocity is controlled by augmenting the variational formulation with suitable Galerkin type terms. Existence and uniqueness of a solution are established for the continuous weak formulation, as well as a semidiscrete continuous-in-time formulation, together with stability bounds and error analysis with rates of convergence. Numerical experiments are presented to verify the theoretical results and illustrate the performance of the method for applications to arterial flow and flow through a filter.

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MS62

Symbiotic Ocean Modeling Using Physics-Controlled Echo State Networks

We introduce the concept of ‘symbiotic’ ocean modelling where high- and low-resolution dynamical models coexist and benefit from each other through data-driven improvements. We specifically focus on how a low-resolution model may benefit from such a symbiotic setup. The broader aim is to improve the e ciency of high-resolution models, while simultaneously enhancing the representation of unresolved processes in low- resolution models. To achieve a symbiosis we use a grid-switching approach together with hybrid modelling techniques that combine linear regression-based methods with nonlinear echo state networks. The approach is applied to both the Kuramoto-Sivashinsky equation and a single-layer quasi-geostrophic ocean model, and shown to simulate short- term and long-term behaviour better than either purely data-based methods or low-resolution models.

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MS62

DNN-MG: Combining Multi-Grid Finite Elements and Neural Networks for eEfficient Flow Simulations

The DNN-MG algorithm complements an efficient multigrid finite element solver with a neural network that represents processes on very fine scales. In contrast to alternative methods, DNN-MG is applicable to arbitrary domains and boundary conditions and generalizes well due to the local operation of the network on a neighborhood of mesh elements. The algorithm was introduced for 2D flow problems where it demonstrated significant speed-ups and high accuracy. Here we present the extension of DNN-MG in two directions. First, we show that the algorithm is also applicable to the considerably more complex problem of 3D flows and that it leads to even larger speed-ups there. Second, we show that transformer neural networks outperform simpler alternatives and in particular provide advantages when the network is applied over a neighborhood of mesh elements instead of the single element. With these extensions, we pave the way for the application of the DNN-MG algorithm to atmospheric and oceanic flows where the neural network can provide a data-driven closure that potentially also incorporates observations.

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MS62

Tailoring data assimilation for models using the discontinuous Galerkinmethods

In recent years discontinuous Galerkin (DG) methods have received increased interest from the geophysical community. In these methods the solution in each grid cell is approximated as a linear combination of basis functions. Ensemble data assimilation (EnDA) aims to approximate the true model state by combining model output with observations using error statistics estimated from an ensemble of model runs. EnDA in geophysical models faces several well-documented issues. In this work we have tested whether it is possible to exploit the DG structure to address three of them. These tests are carried out using a stochastically generated ensemble of synthetic model states. The issues are 1) finite ensemble covariances contain sampling errors that depend on the scales in the solution. It is found that Legendre basis polynomials form a set of wavelets that can be used to remove sampling errors using scale-dependent localisation. 2) Current EnDA requires averaging of dense (satellite) observations and cannot use the information contained in the observations to the fullest. By evaluation of the basis functions, the observation operator can be made to resolve the solution at a sub grid level for higher-order DG schemes. This increases the observation density that the EnDA can effectively digest. 3) Due to its ability to assimilate denser observation sets EnDA is capable of also reducing errors in the 1st-derivative. This is important as these gradients force several physical processes.

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MS62

The Flux-Differencing Discontinuous Galerkin Method Applied to an Idealized Fully Compressible Nonhydrostatic Dry Atmosphere

This talk will discuss the use of higher-order spectral element methods for modeling dry atmospheres. We show that careful choices of numerical fluxes using the Flux-Differencing Discontinuous Galerkin method allow for robust simulations. Furthermore, the natural upwinding afforded by the numerical method allows us to forego explicit dissipation mechanisms utilizing viscosities and diffusivities and solely rely on numerical dissipation. We demonstrate the technique on dry convective boundary layers and climatologically relevant simulations of the atmospheric circulation on a sphere. We conclude by outlining a strategy for incorporating machine learning based parameterizations into spectral element codes.

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MS63

A Multiscale Preconditioner for Darcy Flow

In this talk, a two-level overlapping domain decomposition preconditioner is developed for solving linear algebraic systems obtained from simulating Darcy flow in high-contrast media. Our preconditioner starts at a mixed finite element method for discretizing the partial differential equation by Darcys law with the no-flux boundary condition and is then followed by a velocity elimination technique to yield a linear algebraic system with only unknowns of pressure. Then, our main objective is to design a robust and efficient domain decomposition preconditioner for this system, which is accomplished by engineering a multiscale coarse space that is capable of characterizing high-contrast features of the permeability field. A generalized eigenvalue problem is solved in each non-overlapping coarse element in a communication-free manner to form the global solver, which are accompanied by local solvers originated from additive Schwarz methods but with a non-Galerkin discretization to derive the two-level preconditioner. We provide a rigorous analysis indicates that the condition number of the preconditioned system could be bounded above with several assumptions. Extensive numerical experiments with various types of three-dimensional high-contrast models are exhibited. The research of Eric Chung is partially supported by the Hong Kong RGC General Research Fund (Project numbers 14304719 and 14302620).

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MS63

Flow, Friction, and Contact Mechanics in a Fractured Porous Medium

We study coupling of flow and geomechanics in a fractured porous medium including contact mechanics and friction. We provide a survey of how the mathematical theory of contact mechanics can be used for the fractured medium. This allows consideration of a variety of models being used in the contact mechanics literature to this setting. Further, we include poro-elasticity in a fractured porous medium. The fracture is a lower dimensional surface embedded in a bulk poro-elastic matrix. The flow equation on the fracture is a Darcy type model. The dynamic Biot model is used to describe the coupled flow and geomechanics in porous matrix and is coupled to the fracture flow model. The interface conditions across the fracture includes the contact mechanics and friction effects. The resulting system of equations is a variational inequality coupled to partial differential equations. We prove the well-posedness of this system that include flow, mechanics, fracture flow model and complex friction and contact mechanics. We further consider time discretization schemes where we choose finer time steps for the flow and coarser time steps for the mechanics. We prove the convergence of the iterative schemes for such models. We show how the number of flow steps per mechanics time step influence the convergence rate of the iterative scheme.

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MS63

A Decoupled, Linear, and Unconditionally Energy-

Stable Particle Method for Two-Phase Flows Modeled by the Naiver-Stokes-Cahn-Hilliard System of Equations

In this work, a novel, efficient and unconditionally energy-stable Smoothed Particle Hydrodynamics (SPH) method is proposed and implemented for incompressible two-phase fluid flow modeled by the NavierStokesCahnHilliard system of equations. The idea behind the decoupling scheme is to simplify the calculation into a few linear steps while still maintaining unconditional energy stability. We prove that our SPH method inherits mass and momentum conservation and the energy dissipation properties from the PDE level to the ODE level, and then to the fully discrete level. Consequently and desirably, it also helps increase the stability of the numerical method. Due to its conditional stability, the time step size can be much larger than that of the traditional ISPH methods. Numerical experiments are carried out to show the performance of the proposed energy-stable SPH method for the two-phase flow. The inheritance of mass and momentum conservation and the energy dissipation properties are verified numerically. The numerical results also demonstrate that our method captures the interface behavior and the energy variation process well.

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MS63

Coupled Geothermal Reservoir Simulation and Optimization by Physics-Informed Machine Learning

Heterogeneity and multi-physics nature of the Enhanced Geothermal System (EGS) poses significant challenges in conducting high-fidelity physics simulations, resulting in high computational cost that hinders efficient geothermal management. In this work, a geothermal reservoir management framework is developed by incorporating a low-fidelity yet efficient forward surrogate model based on deep learning with versatile optimizers to expedite the management process. Using a thermo-hydro-mechanical simulation model based on finite element-based reservoir simulation, we parameterized the fracture and well controls and performed THM simulation for EGS, and generate a massive simulation dataset. We trained deep neural network (DNN) architectures with these datasets to predict pressure and temperature dynamics, which are further used to accurately forecast the total net energy harvested from EGS. Instead of conducting the optimization with expensive high fidelity simulations, we directly optimize the well control parameters based on geological parameters to DNN. With DNN being efficient, precise, and fully differentiable, it is able to couple with different gradient-based or gradient-free optimization algorithms to maximize the total net energy by determining the optimal decision parameters. The proposed reservoir management framework demonstrates both efficiency and scalability, which enables each optimization process to be executed in a real-time fashion.

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MS64

A Two-Scale Formulation for Flow in Fractured Porous Media Incorporating Stress-Induced Hysteresis.

We propose a new hydromechanical model for fractured media including hysteresis under loading/unloading conditions to describe fluid withdrawal/injection scenarios more accurately. Such a model is seated on the Barton-Bandis law for joint closure and aims at representing the hysteretic behavior of the joints shown in laboratory investigations during cyclic loading. This yields hysteretic dependence of petrophysical properties on effective stress. The novel approach has enormous potential to impact reservoir management by assisting history matching in scenarios of primary/secondary recovery.

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MS64

Time for Pre-asymptotic Dispersion

We address Taylors complaint about the use of time-dependent dispersion coefficients to model pre-asymptotic dispersion by replacing time-dependence with age-dependence. Age is defined as the contiguous time that solute has endured flow. We demonstrate how this works by application to a recent in-silico experiment addressing the same issue using volume averaging. This experiment is a one-dimensional initial value problem with infinite domain where two sequential (in time) pulses appear within a steady incompressible flow in a pipe. Our approach matches the simulated pre-asymptotic data without additional terms or parameter fitting. The same principle applies to pre-asymptotic dispersion in other important upscaled one-dimensional transports e.g., in river corridor or groundwater flows. Finally a novel closed-form solution is given for the pre-asymptotic dispersion problem in cases where the one-dimensional transport takes place over the whole real line and solute is injected at $x = 0$ as a function of time.

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MS64

Pore-Scale Imaging and Modelling of Coupled Two-Phase Flow and Transport in Porous Media

This talk gives a pore-scale overview of coupled two-phase flow in porous media. 4D X-ray imaging, micromodel optical imaging and pore-scale simulations have been employed to identify the coupled phenomenon how the two-phase fluid configurations impact the transport in porous materials which leads to non-Fickian behaviour.

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MS64

Urban Flooding Open Knowledge Network: Delivering Flood Information to Anyone, Anytime, Anywhere

Floods impact a series of interconnected urban systems (referred to as the Urban Multiplex) that include the power grid and transportation networks, surface water and groundwater, sewerage and drinking water systems, inland navigation and dams, and other systems, all of which are intertwined with the socioeconomic and public health sectors. The Urban Flooding Open Knowledge Network (UFOKN) is an information infrastructure that uses a convergent approach to integrate these multiple interconnected systems, and produce real-time flood forecasts across continental U.S. UFOKN also enables recommendations for routing and evacuation, as well as socioeconomic analysis of the total impact of floods on the Urban Multiplex. The talk will present progress on this multi-organizational project funded by the U.S. National Science Foundations Convergence Accelerator program.

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MS65

A Digital Platform for Integrated Modelling and Optimization of Real Geothermal Storage Plants

Whether for seasonal or short-term storage operations, an underground thermal energy storage (UTES) system stores heat from some source (e.g. waste combustion, industrial cooling system or excess electricity) in the subsurface, for recovery and use later when demand and energy prices are higher. A UTES system may be complex, integrating one or more reservoirs, a number of injection and production wells, heaters, heat pumps and exchangers, all of which must be properly configured and controlled to take into account fluctuating heat supply and demand. Ultimately, the profitability of a UTES system depends not only on the thermal reservoir itself, but on the configuration of surface facilities and the dynamic environment in which it operates. To investigate optimal management of a UTES system using numerical simulation, it is key to have a digital model not only of the subsurface, but of the complete system integrating all the key components of the plant, and data on heat supply, demand and energy prices over time. We here present a digital platform designed for this purpose, developed in collaboration with an industrial partner. Within the framework we present, the UTES plant is described in terms of multiple interconnected loops that are simulated as a fully coupled system. We show how this system can be used to predict and describe the economics of the plant, and provide examples on how the platform can be used in a real industrial setting to optimize its configuration and operation over time.

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MS65

Efficient Nonlinear Solution Strategies for Geothermal Energy Simulation

Geothermal energy systems often exhibit very complex geology, with strong and abrupt variations in geological properties, networks of intersecting fractures, and multiple long, deviating well trajectories. Moreover, the governing equations have very different timescales, with heat rapidly advected through wellbores and fractures, and slowly conducted in the solid rock, whereas mass and energy are strongly coupled through temperature- and pressure-dependent densities. Altogether, this leads to systems of coupled nonlinear partial differential equations that are challenging to resolve numerically. In this work, we show how nonlinear domain decomposition methods can be used to exploit the fact that strong and unbalanced nonlinearities are chiefly localized in space (e.g., near-well regions and fracture networks), and use this to devise efficient nonlinear solutions strategies applicable to practical simulation of geothermal energy systems.

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MS65

Adaptive Learning Acceleration for Nonlinear Solvers Applied to Multiphase Porous Media Flow

We present a machine learning strategy for accelerating the nonlinear solver convergence for multiphase porous media flow problems. The presented method is built on four pillars: compaction of the training space using dimensionless numbers, offline training in a representative simplistic (two-dimensional) model, control of the numerical relaxation (or other tuning parameter) of a classical nonlinear solver, and incremental/adaptive learning to improve the machine learning model in run time (online training). The approach is capable of reducing the number of nonlinear iterations by dynamically adjusting a global parameter (the relaxation factor) based on the physics of the system scaled to a dimensionless space, and by learning on-the-job the specificities of each numerical model. Its implementation is simple and general. In this work, we have also identified the key dimensionless parameters required, compared the performance of different machine learning models, and showed the reduction in the number of nonlinear iterations obtained by using the proposed approach in complex realistic (three-dimensional) reservoir models. We demonstrate that the presented technique dramatically reduces the number of nonlinear iterations without sacrificing the quality of the results, even for reservoir models that are far more complex than the training case.

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MS65

An Efficient Framework for Geothermal History Matching and Prediction Using Adjoint Gradient and Principal Component Analysis

In this study, we present an efficient and flexible adjoint-based framework for history matching and forecasting geothermal production. In this framework, we applied the Principal Component Analysis to reduce the parameter space for representing the complex geological model. The adjoint method is implemented for gradient calculation to speed up the history matching process. Operator-based linearization (OBL) used in this framework makes the calculation of the physical state and its derivatives very efficient and facilitates the matrix assembly in the adjoint method. This study primarily focuses on history matching based on combined observation of well production and in-situ electromagnetic measurements. However, different types of misfit terms can be added to the objective function based on practical considerations. Also, in this work, we propose an optimal weighting strategy for the terms of the objective function to balance their sensitivity with respect to the model control variables. The high efficiency of the framework is demonstrated for the geothermal doublets applied to the heterogeneous geology of the Egg field model with 99 realizations. The framework allows for generating posterior Randomized Maximum Likelihood (RML) estimates of the entire ensemble of the Egg field with a reasonable computational cost. Results show that the framework can achieve reliable history matching results based on the doublets production data and the reservoir electromagnetic measurement.

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MS66

A Mixed-Dimensional Model for Fracture Mechanics Based on the Linear Theory of the Cosserat Poroelasticity

This research was inspired and intended as an extension to the mixed-dimensional poromechanical models for fractured media presented in [1]. There the classical continuum mechanics is considered in the context of finite and infinitesimal strain. We addressed fracture mechanics from a different perspective by considering the linear theory of the Cosserat (micropolar, asymmetric) continuum coupled with a fluid flow problem. Extra regularity can be achieved on the asymmetric component of the stress tensor and fracture tractions through the angular momentum balance defined on surfaces. We addressed the second-order formulation and present numerical results for the adopted model. [1] W.-M. Boon and J.-M. Nordbotten. Mixed-dimensional poromechanical models of fractured porous media, arXiv:2112.05038 2021.

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MS66

A Space-Time Discontinuous Galerkin Method for Wave Propagation in Coupled Poroelastic-Elastic Domains

This work concerns the numerical discretization of wave propagation through coupled poroelastic/elastic materials. Wave propagation is modeled by the elastodynamics equations in the elastic domain and the low-frequency Biots equations in the poroelastic one. The coupling is realized by means of (physically consistent) transmission conditions, imposed on the interface between the domains. For space discretization, we introduce and analyze a high-order discontinuous Galerkin method on polytopal meshes, which is then coupled with a discontinuous Galerkin time integration scheme. We show the stability and error analysis for both semi-discrete and fully-discrete problems. Error estimates are derived in an energy norm. Finally, we present a set of numerical results obtained on test cases with manufactured solutions as well as examples of physical interest.

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MS66

Robust Time-Discretization and Linearization Strategy for PDE-ODE Coupled Hysteretic Flow Problems

In this work, we investigate numerical methods for non-linear parabolic equations coupled to other ordinary differential equations, and/or evolution problems. The diffusion coefficient of the first equation is allowed to vanish (degenerate diffusion) at zero concentration and become singular at full concentration. Such systems model many different physical situations, from the nutrient dependent growth of biofilms, to hysteretic flow of multiple fluids in porous media. We first propose an implicit (semi) time-discretization for the system which is well-posed, consistent, positivity preserving, and satisfies a maximum principle. Then an iterative linearization strategy is proposed to solve the nonlinear time-discrete problems which combines the features of the Newton method and the L-scheme, i.e., a modified L-scheme. The linearization scheme is shown to be globally convergent (even for degenerate and singular cases) provided a Holder continuity result holds for the time-discrete solution. Moreover, it is linearly converging in the non-degenerate case with a contraction rate proportional to a power of the time-step size. Numerical results are presented which corroborates our claims. Furthermore, the performance of the combined scheme is compared to more conventional schemes which reveals that it is significantly more robust and stable than the Newton method, and much faster than the L-scheme.

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MS66

Monolithic Multi-Physics Environmental Simulation Capabilities of the Adaptive Hydraulic Software Suite

Incorporating multiphysics simulations is critical in order to accurately predict environmental dynamics. The Adaptive Hydraulics (AdH) software suite is a high fidelity simulation tool that is capable of solving the 2D and 3D shallow water equations (SW), diffusive wave equation (overland flow), 3D Richards equation (groundwater) and transport applications using stabilized finite elements with fully implicit time stepping. It supports a host of features vital to most hydraulic and transport-engineering applications, including for example, spatial and temporal adaption, surface wave and wind-wave stress coupling, flow through hydraulic structures (weirs, flap gate, etc.) and vessel flow interactions. The AdH suite is also internally linked to a number of process-oriented libraries for cohesive/non-cohesive sediment transport, meteorological forcing and friction and turbulence applications. Recently, the AdH framework was redesigned to allow for monolithic coupling of the softwares internal models. The coupling mechanism is both conservative and easy to implement from a front-end perspective. In this talk we specifically present the coupling framework between (1) AdHs 2D and 3D SW and transport models and (2) AdHs overland flow and groundwater models as well as verification and validation results for both coupled systems.

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MS67

A Novel Numerical One-Domain-Approach (ODA) for Free Fluid and Porous Medium Interaction

Transport phenomena of combined free fluid (ff) and porous medium (pm) flow occur in several industrial, environmental and biological applications. The related mass, momentum and energy transport mechanisms at the ffpm interface have been intensively investigated during the last decades applying formulations at the micro-, meso- and macro-levels. At the microscopical level, the porous medium is assumed as a connected domain of pore spaces filled with the fluid. The flow is governed by Navier-Stokes. At the meso- and macroscopical level, the sets of the governing equations are obtained by averaging or upscaling the equations at the microscopic level over a Representative Elementary Volume (REV). In the present talk, a novel numerical solver for ODA for incompressible and single-phase fluid over a saturated isotropic and anisotropic porous medium is presented. The governing equations, derived by averaging the pore scale microscopic Navier-Stokes equations, are the Incompressible Navier-Stokes-Brinkman equations (INSBEs), discretized over general unstructured meshes. A fractional time step procedure is applied, and a predictor and two corrector steps are sequentially solved inside each time iteration.

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MS67

Interface Conditions for Stokes/Darcy Problems Considering the Symmetric Stress Tensor

Coupled systems for fluid flow in a region containing both free flow and porous medium occur in a variety of applications ranging from engineering to biology to geoscience. A classical example is the flow of water in karst, where the limestone is modeled as a porous medium and the flow in fractures as the free flow. In the free-flow region, we consider the Stokes equations and in the porous domain Darcys law. At the flat interface, these two models are coupled by suitable interface conditions. Recently conditions for the Stokes–Darcy problem allowing arbitrary flow directions to the interface have been derived in (Eggenweiler & Rybak, Multiscale Model. Simul., 2021) via homogenization and boundary layer theory in the case of a non-symmetric stress tensor. Different alternative sets of interface conditions for the Stokes/Darcy case are developed in (Angot, Goyeau & Ochoa-Tapia, Phys. Rev. E, (2017); Angot, Goyeau & Ochoa-Tapia, Transp. Porous Media (submitted), 2021) using volume averaging. In this talk, we present an extension of the interface conditions of (Eggenweiler & Rybak, Multiscale Model. Simul., 2021) for the physically relevant case of a symmetrized stress tensor, entailing a correction for the mass balance equation. We validate these conditions by comparing the simulation results obtained for the coupled problem with the corresponding results at the pore scale. We compare the different coupled models and discuss their abilities and drawbacks.

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MS67

A Hybrid-Dimensional Stokes-Brinkman-Darcy Model for Coupled Free-Flow and Porous-Medium Systems

Coupled free-flow and porous-medium systems have received rising attention in recent years. Such systems appear in many environmental settings and industrial applications. Between the free-flow region and the porous-medium region, there exists a transition region, which severely affects the flow by storing and transporting mass, momentum, and energy. Fluid flow in the thin transition region can be effectively described by dimensionally reduced models. This presentation proposes and analyzes a hybrid-dimensional model for the isothermal and incompressible single-phase flow in coupled fluid-porous systems. We build the hybrid-dimensional model using full-dimensional models in the free-flow and porous-medium regions and a reduced-dimensional model in the transition region. The full-dimensional model consists of the Stokes equations in the free-flow region, the Brinkman equations in the transition region, and Darcy's law in the porous-medium region. The different models are coupled using appropriate interface conditions at the respective two interfaces between free-flow, transition, and porous-medium regions. The reduced-dimensional model is derived by averaging the Brinkman equations across the transition region and formulating suitable closure relations. We analyze the well-posedness of the hybrid system and validate that the model is numerically against the alternative models in the literature.

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MS68

A Macroscopic Model for Unsaturated Flow in Deformable Evolving Porous Media

In this work we derive a model for a deformable porous medium with a growing interface and with phase change to model eco-hydro-mechanical problems in which there is a continuous deposition of porous substrate on the surface and the simultaneous decay and phase change between solid and fluid. The model will then be simplified for one-dimensional scenarios or in multi-dimension under small deformations, leading to a treatable set of equations. The time and length-scales of the problem are discussed and its limiting behaviour is discussed with the help of numerical simulations. Applications to environmental and manufacturing problems are discussed.

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MS68

Multiscale Modeling of Flow and Transport in Graded Porous Media

Understanding of macro-scale fluid flow and transport through heterogeneous porous media has both fundamental and practical importance. Solving flow and transport problems at the pore-scale is not only expensive but also formidable due to the complex geometry of the fluid-solid interface. Thus, researchers have continuously endeavored to propose an effective model that is valid on the macro-scale and incorporates the pore-scale heterogeneities through the transport coefficients. In this study, we proposed the method of multiple scales to systematically upscale the flow of Newtonian fluid carrying a solute through a graded porous media. The main objective of this work is to study how effective permeability and effective diffusion coefficients depend on porosity as well as the geometry of the pore network. We validate our results through rigorous numerical simulations at the pore scale. Finally, we discuss a model one-dimensional filter based on our homogenized equations. Our findings may help in designing efficient filters with application in various industrial processes.

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MS69

Climate Response and Sensitivity: Timescales and

Late Tipping Points

Climate response metrics are used to quantify the Earth's climate response to anthropogenic changes of atmospheric CO2. Equilibrium Climate Sensitivity (ECS) is one such metric that measures the equilibrium response to CO2 doubling. However, both in their estimation and their usage, such metrics make assumptions on the linearity of climate response, although it is known that, especially for larger forcing levels, response can be nonlinear. Such nonlinear responses may become visible immediately in response to a larger perturbation, or may only become apparent after a long transient period. In this talk, I will illustrate some potential problems and caveats when estimating ECS from transient simulations. I highlight ways in which very slow timescales may lead to poor estimation of ECS even if there is a seemingly good fit to linear response over moderate timescales. Moreover, such slow timescale processes might lead to late abrupt responses ('late tipping points') associated with a system's nonlinearities. These ideas are illustrated using simulations on a global energy balance model with dynamic albedo. Also the implications for estimating ECS for global climate models are discussed, highlighting that it is likely to remain difficult to make definitive statements about the simulation times needed to reach an equilibrium.

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MS69

Evaluating Forecasting Systems When Verification-Forecast Pairs are Temporally Correlated

The problem of testing the reliability of forecasting systems is revisited. Depending on the precise nature of the forecasting system, various tools to assess the reliability exist: rank histograms for ensemble forecasts, scores for probability forecasts, spread–skill relationship for mean–variance forecasts etc. In the first instance, these tools mostly provide a qualitative picture only, but they can often be extended yielding quantitative statistical tests for reliability. A general problem with these tests is the assumption of temporal independence of the verification–forecast pairs. This assumption is not even approximately true already in very simple toy examples. In this contribution, a general framework will be presented that allows to take temporal correlations of the verification–forecast pairs into account. More specifically, a refined analysis exploiting the reliability property shows that the test statistics, albeit not independent, still exhibit strong decay of correlations. This property is key to the analysis and is a direct consequence of the reliability property. We demonstrate how this can be exploited to design reliability tests that are rigorously valid under minimal extraneous assumptions.

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MS69

Supermodeling: Improving Predictions with An Ensemble of Interacting Models

Instead of combining data from an ensemble of different models only after the simulations are performed, as in a standard multi-model ensemble, we propose to let the models interact with each other during their simulation. This ensemble of interacting models is called a 'supermodel. In this way, models can compensate for each other's errors before the errors spread to other regions or variables. Effectively, we create a new dynamical system. The exchange between the models is frequent enough such that the models synchronize, in order to prevent loss of variance when the models are combined. In previous work, we experimented successfully with combining atmospheric models of intermediate complexity in the context of parametric error. Here we go beyond, and show results of combining two different AGCMs, different versions of the CAM model, with different resolutions. To combine states from different grids, we convert the individual model states to a common state space with interpolation techniques. We call the combination of different model states a pseudo-observation, and assimilate the pseudo-observations back into the individual models. We apply methods to train the parameters determining the extent and type of information exchange between the models, resulting in a supermodel that outperforms the individual models.

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MS70

Uncertainty Quantification of Density Driven Groundwater Flow

Simulation of salinization of coastal aquifers plays an important role in prediction of availability of drinking water resources. But uncertain fluctuations in hydrogeological parameters may significantly affect the groundwater flow and therefore reduce accuracy of the prediction of the transport phenomena. In this talk, we present numerical approaches for estimation of propagation of the uncertainty from the parameters to the solution in the subsurface density-driven flow models represented by a system of non-linear PDEs. We test them on model problems with random fields for porosity and permeability that represent the limited knowledge of the data. We construct a low-cost generalized polynomial chaos (gPC) expansion surrogate model. Computation of the gPC coefficients is performed by projection on sparse and full tensor grids. Furthermore, we consider a multilevel Monte-Carlo technique (MLMC). Parallelization is applied to both the numerical solution of the deterministic problems (scenarios) and the high-dimensional quadrature over the parametric space. We present results of numerical experiments in 2d and 3d.

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MS70

Robust, Scalable and Adaptive Non-Linear Solvers for Density-Driven Groundwater Flow

Many problems in porous media science and geophysics comprise interactions of processes, and are typically formulated as a system of coupled PDEs. In most cases these systems are transient and often also non-linear. Developing efficient solvers is a delicate task, since one needs to must combine suitable schemes for time integration, linearization, and geometric or algebraic multilevel solvers, which are employed in a parallel computing environment. The effectiveness of the approach is demonstrated for different applications in subsurface flow. These include (i) thermohaline flow, in which density depends on temperature and salt concentration, (ii) thermo-hydraulic flow, which features thawing and freezing in permafrost regions, and (iii) density-driven flow in domains with a free groundwater surface. For these examples, we outline a common solution strategy. We investigate robustness of the numerical methods, develop suitable error estimators and provide scaling results in an HPC environment.

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MS70

Computing Density-Driven Groundwater Flow

The finite volume code df++ (distributed density driven flow), based on the UG toolbox, is used for the modelling of thermohaline groundwater flow in porous as well as fractured media. Free groundwater surfaces are handled using levelset methods. Applications are presented relating seawater intrusion scenarios in coastal areas, regional-scale groundwater flow in granite sites using EPM-approaches and simulations of pollutant transport in a rough lab-scale fracture.

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MT1

Micro-Continuum Modelling: An Hybrid-Scale Approach for Solving Coupled Processes in Porous Media

The micro-continuum approach allows for solving coupled processes including multiphase flow, reactive transport, and poromechanics. It relies on locally averaged Navier-Stokes equations with appropriate subgrid models. Direct applications include systems involving two characteristic pore sizes such as fractured porous media. Micro-continuum approaches for pore-scale were initially designed to compute absolute permeability with image-based simulations accounting for the microstructure that was below the imaging instrument resolution, and, therefore, not observable in the image. Since this pioneering work, the approach keeps growing and the current models handle multiphase flow in the presence of microporosity, displacement of fluid-mineral interfaces along with geochemical reactions (e.g. precipitation and dissolution), and the mechanical deformation as in the swelling of clays. Far from being confined to small-scale systems, micro-continuum approaches are intrinsically multi-scale with the tremendous advantage that they can also simulate processes at the field scale. Hence, a unique system of partial differential equations describes coupled processes in porous media with characteristic sizes ranging from nanometers to kilometers and beyond. In this course, we review the fundamental of micro-continuum approaches and discuss applications of current research interest.

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MT2

Compositional Simulation for Modeling of Complex Subsurface Applications

Thermal multiphase flow and compositional transport in porous media is the base formulation for almost any energy- and environment-related industrial processes. They include hydrocarbon production, subsurface gas storage, advanced geothermal energy production and mitigation of water contamination. In this mini-tutorial, I will describe the main ingredients used in the compositional simulation. I will give an overview of linear and nonlinear solvers, multiphase flash procedures and thermal-compositional extension. I will also present several complex physical phenomena relevant to various industrial applications which require extended compositional simulation.

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MT3

Mesh Refinement/Coarsening Strategies and Advanced Numerical Methods Based on General-Shaped Meshes to Tackle Simulations in Large Scale Discrete Fracture Networks

The objectives of this minitutorial is to share different meshing and numerical strategies that can be combined to tackle simulations in large scale discrete fracture networks. The considered networks will likely contain thousands to more than one million of fractures, following the UFM modeling introduced in Davy et al. (2010). The session will be decomposed into four parts: 1. Efficient mesh generation techniques to handle the complicated geometries arising from the fractures intersections; 2. Agglomerations strategies to enable coarsening possibilities and efficient generation of polygonal meshes; 3. The Hybrid High Order (HHO) method and its a posteriori error analysis 4. Illustrations on several examples of the benefits of the combination of efficient mesh generation, HHO and adaptive mesh refinement strategies in the context of single-phase flow simulations in large scale discrete fracture networks.

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MT3

Mesh Refinement/Coarsening Strategies and Advanced Numerical Methods Based on General-Shaped Meshes to Tackle Simulations in Large Scale Discrete Fracture Networks

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MT3

Mesh Refinement/Coarsening Strategies and Advanced Numerical Methods Based on General-Shaped Meshes to Tackle Simulations in Large Scale Discrete Fracture Networks

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PP1

Advanced Statistical Learning Algorithms for Comparative Multisource Formation Permeability Modelling

For accurate prediction of formation permeability in non-cored intervals, three algorithms were adopted for comparative core permeability modelling given multisource-multiscale measurements of well logs and core data: Shale

Volume, Neutron Porosity, Water Saturation, and Rock Lithofacies. The algorithms are Multiple Linear Regression (MLR), Multivariate Adaptive Regression Splines (MARS), and Generalized Boosted Modelling (GBM). GBM has resulted in much more accurate modelling and prediction of formation permeability by achieving the Least Root Mean Square Prediction Error.

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PP1

A Posteriori Error Estimate for the Thermo-Poroelasticity Problems; Simulated by Modified Method of Characteristics and Enriched Galerkin

We consider modeling the time-dependent thermo-poroelasticity problems by the method of characteristics for the energy balance equation, Enriched-Galerkin for fluid flow, and continuous Galerkin for mechanics. A posteriori error analysis of this discretization is performed for the coupled multiphysics system and shows optimal convergence rates. The error estimate establishes lower and upper residual-based bounds for the discretized solution. The coupled system is simulated with MOOSE finite element simulator. MOOSE discretization and adaptivity capabilities are extended to simulate the thermo-poroelasticity problems along with its error estimate. The developed error estimate was used for modeling several porous media analytical and experimental problems with an efficient spatial and temporal adaptivity strategy. Numerical results confirmed the enhancements and savings in computational cost gained compared to conventional finite element discretization schemes.

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PP1

Mixed-Dimensional Model for Simulation of Reactive Transport in Fractured Porous Media

Numerical simulations of reactive transport in fractured porous media are necessary for several environmental and engineering applications. Networks of fractures may behave as shortcuts for the transport processes, whereas chemical reactions trigger mineral dissolution and precipitation that alter the porous medium and fracture walls locally. This will either cement flow paths or open new ones, impacting the global flow regime. Here, we present an approach to simulate reactive transport in fractured porous media, where dissolving and precipitating minerals might alter the flow characteristics. Our numerical solution strategy is based on a discrete fracture-matrix model with a mixed-dimensional representation of the fractured media. The model equations consist of coupled partial differential equations for the fluid flow, heat transfer and solute transport, and non-linear algebraic equations representing the chemical reactions. The partial differential equations are discretised using finite-volume methods, and the resulting non-linear system of differential-algebraic equations is solved by Newtons method. Numerical tests illustrate our models ability to capture the tightly coupled physical and chemical processes. Moreover, we discuss application of our framework to simulations representative of, e.g., geothermal field cases, where computational cost becomes a major concern.

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PP1

Optimising the Choice of Parameters in Marine Biogeochemical Models

Ocean biogeochemical models (OBGCMs) are complex mathematical representations of the interactions between geophysical, chemical, and biological tracers in the ocean, such as carbon and phytoplankton. These models are very important in the study of a variety of phenomena, such as the ocean carbon cycle, and are now an integral part of CMIP-like Earth System Models used in climate prediction. In general, the governing dynamical equations of OBGCMs are mostly empirically derived and contain several parameters that must be calibrated. The calibration of these parameters has been historically carried out via a "trial-and-error" approach: this consists of trying out a few ad-hoc chosen values by hand, until the model reasonably reproduces a chosen set of observations, in what is usually a very time-consuming process overall. As increasing quantities of high-resolution global data for tracers become accessible, combined with a growth in high-performance computing power available, it has become possible to tune the model computationally using mathematically robust and algorithmically efficient optimisation methods. In this work, we will present and discuss two emergent optimisation techniques, namely the Covariance Matrix Adaptation Evolution Strategy (CMA-ES) and the Derivative-free Optimisation by Least Squares (DFO-LS) methods, which can be used to fit parameters for global OBGCMs. We will also illustrate this approach with a few computational results.

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PP1

Incorporating Geological Structure into Sensitivity Analysis of Contaminant Transport Modeling

Simulating subsurface contaminant transport at the kilometer-scale often entails modeling reactive flow and transport within and through complex geological structures. These structures are difficult to mesh and as a result geologic structure is typically represented by one or a few deterministically generated meshes for uncertainty studies. Uncertainty in geologic structure can have a significant impact on contaminant transport and should be fully incorporated within uncertainty quantification (UQ) and sensitivity analysis (SA) for subsurface contaminant modeling. An open-source modeling framework is used to perform a

sensitivity analysis on transport of I- 129 from a hypothetical radioactive waste repository in a shale host rock with uncertain geologic structure. Four uncertain flow parameters are sampled in addition to realization of the geological structural model in a nested SA/UQ analysis. Concentration of I-129 at monitoring points downstream of the repository are used as the quantities of interest for determining model sensitivity to input parameters. We discuss the results of this study as well as challenges faced while incorporating geological structure into large scale UQ/SA studies of contaminant transport modeling. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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PP1

Predicting PFAS Leaching in Heterogeneous Vadose Zones

PFAS are emerging contaminants widely dispersed in the environment. In particular, many field investigations demonstrate that significant amounts of PFAS accumulate in vadose zones and are migrating downward to contaminate groundwater. Recent laboratory and mathematical modeling studies have consistently shown that PFAS experience strong retention in the vadose zone due to interfacial partitioning at airwater and solidwater interfaces. However, most of the investigations to date focused on homogeneous vadose zones that underrepresented the impact of heterogeneitya primary factor known to dominantly control the subsurface transport of many contaminants. We present a comprehensive modeling study to quantify how heterogeneity-generated preferential flow accelerates PFAS leaching to groundwater. 2D and 3D simulations of PFAS leaching in stochastically generated heterogeneous vadose zones show that while short-chain PFAS experience enhanced leaching similar to non-surface-active contaminants, long-chain PFAS undergo unique accelerated leaching that is greatly amplified due to reduced air-water interfacial areas along preferential flow pathways. Our modeling analyses highlight the criticality of characterizing and representing subsurface heterogeneities for accurate predictions of PFAS leaching in heterogeneous vadose zones.

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PP1

Geomechanical Modeling of Deformation Banding in the Navajo Sandstone, San Rafael Monocline, Uta, Usa

Deformation bands are ubiquitous geological features in many types of rocks. Depending on their micro-structure, they can act as conduits or barriers to fluid flow. Understanding their origin and characteristics relating to the host rock properties and their depositional and structural-geological history is important. We present a forward-modeling technique based on the geomechanical Bifurcation Theory (BT) to predict the formation of deformation bands in sandstone. According to BT, the formation of deformation bands results from strain location, which in turn stems from instability in the stress-strain response of materials during loading. Due to bifurcation, a material that undergoes homogeneous deformation can reach a point at which the material experiences instability and deformation becomes non-homogenous. We implemented BT in the commercially available geomechanical code FLAC (Fast Lagrangian Analysis of Continua). We applied it in the field-scale modeling of deformation banding in the Navajo Sandstone in the San Rafael Monocline in Utah induced by fault propagation folding. The results show that geomechanical modeling using BT has a powerful potential to simulate the physical processes in forming deformation banding in rocks. Predicted deformation bands, specifically the pervasive bedding-parallel bands in the Navajo sandstone formation, normal faulting in the upper limb, and reverse faulting in the lower limb, generally agree with field observations.

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PP1

Application of the Transient Drainage Volume to Fractured Well Test Interpretation

Fractured wells have become ubiquitous in the development of petroleum reservoirs, especially for unconventional resources. However, as multi-stage hydraulic fractured wells have moved to tighter fracture spacing and more complex fractures, the interplay between reservoir linear flow for each fracture, finite conductivity of each fracture, and the interference between fractures has made the interpretation of field data more difficult. In the current study we present, validate and apply three new analytic models for fractured well performance based upon the concept of the transient drainage volume. (1) Infinite conductivity fracture solutions that interpolate between linear flow at early time, and mid-time radial flow. (2) Finite conductivity corrections that interpolate between bi-linear flow and the infinite conductivity solution. (3) Multi-stage hydraulic fractured well solutions based on the finite conductivity solution but that develop approximate boundary dominated flow, replacing the radial flow signature of a single fracture. The solutions are rapid to evaluate and provide novel solutions that may be used for the inversion of production or well test data to determine formation permeability, fracture area, hydraulic fracture conductivity, and the SRV volume.

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PP1

DeepWaves: Next Generation Modeling, Simulation, AI, and Data Analytics for Efficient Natural Resources Exploration

The mineral and hydrocarbons exploration industry face significant challenges in discovering untapped resources while simultaneously keeping exploration costs in check. We present the DeepWaves project, a novel approach that aims to address these challenges by leveraging advanced computational modeling, simulation, machine learning, and artificial intelligence techniques. We have developed novel computational models and machine learning (neural networks) techniques to seismic imaging to enhance exploration efficiency while reducing exploration and operational costs. The technology can help speed up the exploration phase, locate untapped pockets of oil and gas, and mineral deposits, leading to more new discoveries. Ultimately, our approach and project has the potential to revolutionize the exploration process for the oil & gas and mining industries and could significantly impact future energy and natural resources worldwide.

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PP1

Voronoi Or Hexahedral Meshing for Simulation Accuracy and Speed?

In large-scale simulations of fluid flow through subsurface porous media it is frequently necessary to flex hexahedral meshes to conform to geological and engineered features. However, in regions where grid cells are irregular, the poor quality of the mesh can negatively impact the accuracy of the simulation, even in very simple models. One alternative to simulating on flexed hexahedral meshes is to use Voronoi unstructured polyhedral meshes. By construction, Voronoi meshes have only orthogonal fluxes between cells, and unstructured meshes do not systematically bias the flow field, reducing two important sources of numerical error. However, unstructured polyhedral meshes significantly increase simulation time due to the computational cost of solving a dense, unstructured Jacobian matrix. A series of one- and two-phase analytical benchmark problems are simulated on hexahedral, flexed-hexahedral, and unstructured Voronoi meshes using the finite volume simulator PFLOTRAN. The accuracy of simulated results and computation times are compared for each of the cases. The results demonstrate cases where it is imperative to use unstructured meshes to obtain an accurate solution, and cases when Voronoi meshes are likely not worth the additional computational cost. Finally, simulated results of two-phase flow on flexed hexahedral and Voronoi meshes on a model with geological features are compared. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

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PP1

Development and Testing of a Well Model for Performance Assessment at the Waste Isolation Pilot Plant (wipp)

The Waste Isolation Pilot Plant (WIPP) in southeastern New Mexico is the U.S.s only operating deep geologic repository for defense-generated transuranic radioactive waste. Performance assessment (PA) for the WIPP is designed to evaluate the potential for consequential radionuclide release during a 10,000-year post-closure period using a probabilistic approach. We have developed a wellbore flow and transport model in the high-performance subsurface simulator PFLOTRAN which can solve for flow and transport in a well without meshing it into the reservoir, which can improve simulation time. The wellbore model solves a fully implicit 1D, 2-phase flow step coupled sequentially to a transport step including radioactive decay and ingrowth. The wellbore automatically meshes a variable-resolution grid, it can be cased over any segment, and physical properties can be assigned to any well segment (e.g., concrete plugs). Users can control the well-reservoir exchange model and the wellbore numerical convergence criteria. The wellbore model is sequentially coupled with the reservoir flow and transport solutions, which is computationally efficient but can be numerically challenging. Wellbore model adaptations to ensure adequate convergence include an option to declare steady-state in the well and an adaptive source/sink term to restrict pressure oscillation. We present these numerical techniques and a suite of verification tests demonstrating simulator performance. SAND2022-16878A

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PP1

Using Physics-informed Neural Networks to Simulate Solute Transport in Heterogeneous Mediums with Uncertain Architecture

Subsurface porous systems are often composed by multiple geomaterials in an uncertain internal architecture, which leaves us with an incomplete knowledge about properties driving subsurface flow regimes. Addressing the uncertainty arising from geometrical scheme of the subdomains is of high importance in subsurface contaminant transport. We adopt a continuum-approximation of the transport process and we rely on Deep Learning based PDE solvers, which highly simplify time-consuming steps such as space-time discretization. Recent works show that Physics Informed Neural Networks (PINNs) is a promising technique for using structured prior knowledge to build data-efficient solvers. We will explore application of these weakly supervised methods to solution inference of contaminant transport problems in heterogeneous porous media, where limiting challenges arise. Then we will employ adaptive activation functions and domain decomposition techniques, to gain control over smoothness of solution, and for partitioning the PDE problem into several subdomains, respectively. The latter allows us to exploit PINNs for heterogeneous systems, while the solution continuity across the various sub-network models is maintained by enforcing flux continuity via appropriately designed loss functions. Finally, we will go over the main pros and cons of PINNs when compared to conventional solutions.

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PP1

Advanced Solvers for Simulating Multiphase Flow and Transport Within Large-Scale Engineered Subsurface Systems

Modeling large-scale engineered subsurface systems entails significant numerical challenges. The US DOE Waste Isolation Pilot Plant plans to employ 3D simulation models to modernize performance assessment for the regulatory period of 10,000 years. The challenges arise from: (a) the need to refine the discretization to accurately represent repository while modeling large-scale flow and transport processes throughout geological formations; (b) the strong contrast in porosity and permeability; (c) the nonlinear constitutive relations for multiphase flow; and (d) radiolysis, iron corrosion, and biodegradation processes generating gas which may dry out portions of the repository. These can each lead to an ill-conditioned Jacobian matrix and poor convergence within Newtons method due to discontinuities and/or nonlinearities in constitutive models. We apply the open-source simulator PFLOTRAN which employs a finite-volume discretization and uses the PETSc parallel framework. We evaluate the performance of preconditioners for the multiphase flow equation including constrained pressure residual (CPR-AMG) preconditioner for Newton-Krylov, and we implement, within PETSc general-purpose nonlinear solvers, Newton trust-region dogleg Cauchy (NTRDC) to demonstrate improved efficiency. The flow and transport simulations show up to 50 times speed-up compared to PETScs default solvers. Moreover, these solvers enable the completion of challenging scenarios that were previously impossible.

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PP1

Hierarchical Modeling of Wildfire Spread

The dynamical behavior of wildfire can be described by coupled (partial) differential equations. The literature deals in two main approaches with the model: On the one hand, there are rigorous mathematical proofs for submodels including less of the mechanisms. On the other hand, numerical simulations show exemplary behavior of the full model in complex settings. A special property of the model is an unsteady reaction function for the combustion process, starting at a certain temperature. We present recent results in the gap between the two approaches. Further, the model shows transport or diffusion dominated behavior depending on the wind speed. We prove analytical results estimating the remaining biomass and develop conditions for stopping the spread of the fire. Numerical simulations support and extend those findings.

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PP1

Instantaneous Physics-Based Ground Motion Maps Using Reduced-Order Models

The computational cost of realistic numerical simulations of wave propagation complicates their applicability to problems that need real-time solutions (e.g., earthquake early warning) or many solutions for different earthquake sources, (e.g., probabilistic seismic hazard assessment). Here, we present a reduced-order model (ROM) that instantaneously generates peak ground velocity (PGV) maps. The ROM considered is the interpolated proper orthogonal decomposition (POD). We use high-resolution 3D seismic wave propagation simulations as a full-order model resolving up to 2 Hz and analyze two scenarios consisting of a flat 1D layered and 3D velocity models that includes topography. We quantitatively compare four function approximators with POD: radial basis function (RBF) interpolation, multilayer perceptron neural networks, random forests and k-nearest neighbors. RBFs are the most accurate approximator, resulting in ¡ 0.1 cm/s average PGV error when applied to an independent testing dataset. We predict PGV maps for 1 million different focal mechanisms, in which the ROMs identify potentially damaging ground motions that might be overlooked when using only a few physics-based simulations. We quantify correlations between focal mechanism, depth, and accuracy of the predicted PGV. Lastly, we extend Rekoske et al., arXiv:2212.11335, by further considering error-driven adaptive sampling in parameter space and time dependent objective functions.

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PP1

Error Analysis for Discontinuous Galerkin Semidis-

cretization of Degenerate Parabolic Problems

We study an error analysis of the time-continuous semidiscrete scheme for nonlinear parabolic equations admitting fast-diffusion type of degeneracies. A typical example of such a differential equation is Richards' equation, widely used to model the fluid flow in porous media. The solutions to this problem usually lack regularity, and they have been studied in papers on the existence, uniqueness, and regularity of solutions to elliptic-parabolic differential equations. Due to the nonlinear diffusion, we employ the incomplete interior penalty Galerkin (IIPG) method for spatial discretization. Since the considered problem has an extra nonlinearity, namely, in the accumulation term, special techniques for numerical analysis of the scheme are required. We use continuous mathematical induction to prove a priori error estimates in the L^2-norm and the so-called DG-norm with respect to spatial discretization parameter and the Holder coefficient of the accumulation term derivative.

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PP1

Global Synchronization of Octonion Valued Neural Networks with Unbounded Time Varying Delays.

The article investigates the global exponential and adaptive synchronization of octonion-valued Neural Networks (OVNNs) with unbounded time-varying delays. On behalf of two different types of controllers, namely feedback and adaptive control, several fruitful criteria are obtained to ensure the global synchronization of OVNNs. This work is followed by a non-separation approach, contrary to results on OVNNs adopted the method in which OVNNs are separated into eight equivalent real-valued neural networks due to overcoming that the OVNNs are non-commutative and non-associative. Because of the non-separation approach, this work is compact and more concise, making it easier to deal with OVNNs. Authors of the present study also consider unbounded delays because neuron behavior relates to its entire past. Finally, two numerical examples are given to demonstrate the efficiency and effectiveness of the proposed result and the application of OVNNs to associative memory to demonstrate their capacity to accurately retrieve true color image patterns.

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PP1

Interection of Shear Wave on Semi-Infinite Moving Crack under Antiplane Shear Loading

The article deals with the study of a moving interfacial semi-infinite crack situated between two orthotropic strips of different composite materials. The crack surface is under the shear wave disturbance. The governing equations have been solved by applying the Fourier transform technique to get the desired standard form of the Wiener-Hopf Equation, which is further solved by using the Wiener-Hopf Method. The analytical asymptotic expressions for physical quantities like Stress Intensity Factor(SIF) and Crack Opening Displacement(COD) for the crack have been obtained. The nature of SIF and COD for different combinations of composite materials and also for various depths of the semi-infinite strips have been depicted graphically.

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PP2

Pattern Recognition for Extreme Events

While extreme climate events are becoming more frequent, their impact, i.e. the level of devastation they cause, is intensifying. Current models project even more intimidating scenarios. In this respect, we aim to develop a pattern recognition framework of extreme events. For detection of potentially spurious and informative behaviour leading to an extreme event we will use spectral analysis tools. We will extend the nonparametric spectral estimation method, called singular spectrum analysis (SSA) [Broomhead, D.S., King, G.P. Extracting qualitative dynamics from experimental data, 1986] by focusing on the evolution of the eigenvalues. The main result of the SSA method is the reconstructed signal. However, we will also investigate the byproducts (such as eigenvalues, noise, etc) as well as the relationship between the SSA modes. Additionally different covariance matrices will be considered for embedding phase.

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PP2

A Critical Assessment of the Finite-Volume-Based Embedded Discrete Fault Mechanics Method (sEFVM)

The smoothed enhanced finite volume method (sEFVM) was developed for simulating deformation of porous faulted media. This method is flexible in allowing independent computational grids for the faults and the matrix and placing only one additional degree of freedom per fault element. The use of finite volumes allows for the calculation of locally conservative mass flux and stress fields. sEFVM solves for matrix deformation and fluid pressure in a fully-implicit coupled manner and the fault slip with sequential-implicit coupling. A post-processing smoothing step is included to ensure smooth slip profiles. The accuracy of sEFVM was tested for various 2D cases consisting of faulted reservoirs with offsets, undergoing compaction and pressure depletion. The results show sEFVM is accurate for smooth stress profiles however deviations exist for discontinuous stress profiles. We are working on developing a hybrid method by integrating the analytical solution with sEFVM.

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PP2

Bridging the Gap Between Lab Experiments and Mixed-Dimensional Modeling for Flow in Fractured Media

The existence of fractures in porous media has a strong impact on the characteristics of the flow behavior. In geological rocks, fractures occur both naturally as well as intentionally induced as in geothermal applications. Thus, accurate modeling and simulation of flow and transport in fractured media is vital for many industrial applications. Mixed-dimensional models have been widely used for modeling flow in fractured media. The high aspect ratio of the fracture width as compared to their remaining dimensions allows for representing them as lower-dimensional manifolds. By combining mass conservation and Darcys law on each subdomain and mass transfer between domains, underlying equidimensional models can be conveniently replaced. Yet, despite the large interest in mixed-dimensional models for flow in fractured media, direct comparisons to high-quality lab experiemnts have been missing. On this poster, we present such a comparison study based on PET experiments of tracer transport in fractured sandstone and corresponding numerical simulations (using PorePy). In addition, we present tailored functionality of an open-source image analysis toolbox (DarSIA) used to transfer PET images to Darcy-scale images and to compare different Darcy scale images from different origins by suitable metrics.

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PP2

Data-Driven Optimisation Algorithms for Local Dynamic Model Adaptivity

We develop a data-driven optimisation-based adaptive model for gas storage scenarios which couples a Vertical Equilibrium Darcy-model with a full-dimensional Darcy-model. The Vertical Equilibrium model is founded on simplified physics, being the instant segregation of, in our case, two phases, and offers a trade-off between accuracy and speedup while the full-dimensional model emphasizes on accuracy over speed. Based on a custom criterion, our algorithm automatically deduces where the simplified model can be utilized while maintaining a high level of accuracy and where the full-dimensional model is necessary. All this is based on the work of [Beatrix Becker, An Adaptive Multiphysics Model Coupling Vertical Equilibrium and Full Multidimensions for Multiphase Flow in Porous Media, 2018]. In the past, we have used the IMPES method for solving the system of partial differential equations. However, by investigating a fully implicit, coupled model, we hope to achieve an overall speedup, especially in scenarios where capillary forces or non-linear quantities in general dominate. With hydrogen being a prominent energy carrier, we would like to contribute to an effective and efficient model for predicting the flow and spread of hydrogen in subsurface aquifer storages.

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PP2

First Steps Toward Performance Portable Algorithms for Shallow Water Equations on Unstructured Grids

We present our discontinous Galerkin (DG) finite element implementation for the shallow water equations. In the focus of our work is the performance portability between CPUs, GPUs and FPGAs using a common code base. To achieve this goal, we use the SYCL programming model. The FPGA port of the original implementation has been ported to SYCL. This SYCL implementation serves as the first step towards a performance portable implementation, as it runs with reasonable performance on CPUs and GPUs – without needing hardware specific code.

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PP2

Serghei: An Hpc Enabled Shallow Water Solver for Hydrological Applications

The Simulation EnviRonment for Geomorphology, Hydrodynamics and Ecohydrology in Integrated form (SERGHEI) model framework is a multi-dimensional, multi-domain and multi-physics model framework for environmental hydrodynamics, ecohydrology, morphodynamics, and, importantly, interactions and feedbacks among such processes. The hydrodynamic core is a shallow water solver (SERGHEI-SWE) harvesting robust and efficient numerical schemes based on augmented Riemann solvers and implemented in a performance-portable HPC fashion. SERGHEI is built on the Kokkos programming model, allowing it to transparently operate on CPU-based systems and heterogeneous systems based on GPU accelerators. We present the SERGHEI model framework, focusing on its first operational module SERGHEI-SWE, designed to be applicable to hydrological, environmental and consequently Earth System Modelling problems, but also to classical engineering problems such as fluvial or urban flood modelling. We discuss the performance of the solver on well-known benchmarks and on large-scale hydrological simulation and flooding problems, in particular showing its scalability and performance-portability in several TOP500 HPC systems. We show that SERGHEI-SWE is capable of efficiently running on hundreds of scientific-grade GPUs, thus enabling high-resolution surface flow simulation for very large domains.

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PP2

Large-Scale Reactive Transport Joint Inversion of Head and Concentration Data: a Benchmark on Deterministic and Stochastic Approaches.

In the context of Reactive Transport, this work presents a benchmark on three well-known large-scale parameter estimation approaches. The first one is deterministic and relies on a quasi-newton solver coupled with an efficient gradient computation through the adjoint state. The second one, the Principal Geostatistical Approach (PCGA) is a ”gradient-free” geostatistical inversion strategy based on covariance matrix compression through a randomized eigen decomposition. Finally, the Ensemble Smoother with Multiple Data Assimilation (ESMDA), another stochastic ”gradient-free” approach relies on initial ensemble of estimated parameters realizations. The three approaches are compared on two applications. The first application is a steady state hydraulic tomography using sequential pumping tests and a joint inversion using hydraulic head and tracer test data. The second application is a three-dimensional uranium in situ recovery case on synthetic and real data. The performance of the three algorithms to match the data are compared, as well as practical pros and cons: number of runs needed, memory consumption, prior knowledge required. Insights from uncertainty analysis are also discussed getting a better understanding of the reliability of each method.

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PP2

Generalized Coupling Conditions for Fluid-Porous Systems: Validation and Efficient Solution Strategies

Coupled free-flow and porous-medium systems with arbitrary flow directions to the fluid-porous interface appear routinely in environmental settings and industrial applications. Traditionally used coupling approaches, which are based on the Beavers-Joseph interface condition, are valid only for uni-directional flows parallel or perpendicular to the interface. In recent years, several alternative coupling concepts have been proposed for arbitrary flow directions to the fluid-porous interface. However, some of them are only theoretically derived and not validated yet. Moreover, efficient solution strategies are developed for coupled fluid-porous problems with the classical set of interface conditions. In this presentation, we validate and compare several generalized coupling conditions for arbitrary flow directions and propose preconditioners to solve the resulting coupled problems efficiently.

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PP2

Pore-Scale Insight of Hydrogen Transport in Porous Media

Underground Hydrogen Storage (UHS) using porous formations has great potential as a large-scale (TWh) energy storage technology. To ensure the efficiency of the storage operation, it is essential to employ multiscale modeling and simulation strategies that study the micro-scale physics and derive input parameters for the continuum-scale dynamic models. To properly characterize the dynamics of the system and study this complex process at the pore-scale, the present study compares a dynamic pore-network modeling (D-PNM) approach with a quasi-static pore-network modeling. The goal is to simulate the immiscible two-phase flow of hydrogen and water through a pore network model of a porous structure. The model input parameters are based on the experimentally obtained fluid-gas properties as presented in the literature. As for the rock, statistical pore network models are generated to mimic the digital network information which is based on 3D

X-ray images of porous samples. The developed D-PNM solves the transient multi-phase Stokes equations fully implicitly for pressure and phase volume concentrations, to preserve simulation stability. Through several test cases, the transport characteristics of the hydrogen/water interface are analyzed. These results critically assess the validity of quasi-static pore network modelling in the application of UHS and provide new insights on how a representative continuum-scale model should be created to study the process at the field scale.

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PP2

Three-Dimensional Hydrodynamic Modeling of Microplastic Transport in Lakes and Reservoirs

A three-dimensional hydrodynamic and microplastic transport model was set up to simulate the transport and fate of different types of microplastic particles in the reservoir Groer Brombachsee, Germany. The simulations were conducted using Delft3d FM (Flexible Mesh). Particle transport was simulated with an Eulerian approach adapting the sediments and morphology module. First results for horizontal and vertical distribution patterns of particles of different sizes and densities are available for two different in- and outflow regimes of the reservoir. It was found that both particle density and size strongly influence the distribution of microplastic in the computational domain. While smaller lighter particles distributed along the whole horizontal extent of the reservoir, particles with higher density or larger size settled within a delimited area around the inflow location which indicates a significantly higher settling velocity.

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PP2

Successive Approximations for Fractional Bvps with Non-Local Boundary Conditions

Over the past few decades, fractional differential equations have gained popularity among scientists aiming to create realistic models of complex real-world phenomena. The main advantage of fractional operators is their ability to capture non-local and memory effects, which are significant in many physical processes, such as fluid flow through porous media, viscoelasticity, and anomalous diffusion. The non-local nature of such phenomena can be modeled as fractional boundary value problems. Exact solutions are often unavailable, which has prompted the development of approximation methods. In the present work, we consider the existence and uniqueness of solutions to a system of nonlinear fractional differential equations, subject to integral boundary conditions. We apply a numerical-analytic technique to construct a sequence of successive approximations and prove its convergence to the exact solution of the boundary value problem. The nonlocal boundary conditions are dealt with via a parametrization. The convergence of the technique is improved and its applicability is extended to a wider class of problems using a dichotomy-type approach. The behavior of the approximate solutions is governed by a set of parameters, whose values are calculated numerically. Our results are applied to a fractional order problem, which in the case of the second order differential equation models the flow of the Antarctic Circumpolar Current.

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