IP1

Frontiers of Decision Making in Large Companies (Cleaning Up After the Laureates)

Over the past 200 years our view of human rationality has moved from "perfect' (Adam Smith) to "bounded" (Herbert Simon, Nobel Laureate 1978) to "biased" (Daniel Kahneman - Nobel Laureate 2002). Unfortunately the Laureates left two practical questions unanswered: a) how bad is our decision making, and b) how do we make better decisions? This talk addresses these two questions from an Intel perspective. I will give a brief overview of decision support tools at Intel over the past 20 years (addressing boundedness) the benefits from which can be used to set a lower bound on how bad we are. Then I will describe our recent projects to improve decision making (addressing biases) including applications of "wisdom of crowds" and "decision markets".

Karl Kempf
Intel Corporation
karl.g.kempf@intel.com

IP2

The Ongoing Challenge Improving Organizational Performance with Better Decisions

Organizations, from health care facilities to manufacturing giants, can be viewed as an ongoing sequence of loosely coupled decisions where current and future assets are matched with current and future demand across the demand-supply network at different levels of granularity ranging from placing a lot on a tool to a five-year capacity plan. Every organization has as a stated goal to make smarter decisions. However, each decision is a result of a complex interaction between process (culture), data, and the models (math) used. The net result is an ongoing challenge for the math guys to (a) find the right models and (b) navigate the political terrain – if Ptolemys theory of circle of circles explains movement of planets, why bother with Kepler, Newton, gravity, elliptical orbits, and calculus. This presentation will cover some recent applications at IBM manufacturing that upset the social order.

Kenneth Fordyce
IBM Systems and Technology Group
fordyce@us.ibm.com

IP3

The Application of Numerical Modeling to Hydrocarbon Exploration Using Controlled Source Electromagnetism

This talk will outline the development over the last ten years of a new approach to hydrocarbon exploration based upon the application of electromagnetic methods in the deep water marine environment. A key component of this new technology to be highlighted in this talk is the application of accurate numerical modeling to predict and interpret the electromagnetic response of complex, fully three dimensional, models of subsurface resistivity. Time domain measurements, designed to produce responses targeted to specific frequency ranges (0.01 to 10 Hertz), made in deep water conditions demonstrate that active source electric field responses contain noise components at the unusually low level for geophysical measurements of approximately one part in ten to the fourteenth power. This low noise level permits the relatively small perturbations in electric field patterns caused by thin resistive anomalies arising from hydrocarbon saturated reservoirs to serve as a reliable direct hydrocarbon indicator complementing other techniques based upon seismic methods. Numerical solutions of Maxwells equations governing realistic subsurface situations are accomplished using finite difference and finite element techniques applied to basin scale models of sufficient size to capture the electromagnetic response of resistivity structures associated with water bottom topography, salt diapirs and sedimentary layers. In spite of the significant progress made possible by the advent of cost effective symmetric massively parallel computing platforms, a number of potentially promising avenues of further development remain. Among these are: the development of practical advanced multi-grid methods, pre-conditioners well suited to symmetric parallel implementation, solution techniques appropriate to high resistivity contrast situations and developments in gradient based optimization designed to accelerate the slow convergence observed in electromagnetic imaging. These issues will be illustrated with an eye toward stimulating further work in these areas by the applied mathematics community.

James Carazzone, Kenneth Green
Exxon Production Research Company
jim.j.carazzone@exxonmobil.com,
ken.e.green@exxonmobil.com

IP4

Mathematics in Modeling and Simulation: Evolution and Issues

In this address we will discuss the changing role of mathematics in modeling and simulation. Mechanical engineering projects have always used modeling and simulation to understand, predict, and control what the project will eventually produce and how it will behave and perform: model ships and towing tanks are used to understand sea keeping properties of naval vessels, model airplanes and wind tunnels are used to understand flight properties of airplanes. The notion of building a model and then simulating its performance is not new. What is new is the use of mathematical models and computer aided engineering (CAE) tools for simulation, understanding, and eventual design. But the emphasis on mathematical modeling and the use of CAE tools raises a host of issues that are beyond the domain of engineering, issues that need to be resolved by mathematicians. In this talk we will follow the evolution of design and the connection with mathematics through the 20th century with an eye to highlighting and understanding aspects of modern design methodology that belong uniquely to the mathematical domain and are differentiated from the engineering domain.

David R. Ferguson
Access Analytics
david.r.ferguson@comcast.net

Thomas A. Grandine
Applied Mathematics
The Boeing Company
thomas.a.grandine@boeing.com

IP5

Mobility, Data Mining and Privacy: Lessons from the GeoPKDD EU Project

The technologies of mobile communications and ubiquitous computing pervade our society, and wireless networks sense the movement of people and vehicles, generating large volumes of mobility data. This is a scenario of great opportunities and risks: on one side, mining this data can produce useful knowledge, supporting sustainable mobility and intelligent transportation systems; on the other side, individual privacy is at risk, as the mobility data contain sensitive personal information. A new multidisciplinary research area is emerging at this crossroads of mobility, data mining, and privacy. The talk assesses this research frontier from a data mining perspective, and illustrates the results of a European-wide research project called GeoPKDD, Geographic Privacy-Aware Knowledge Discovery and Delivery,funded by the EU Commission under the FET-Open program. Particular attention will be placed upon privacy-aware geographic knowledge discovery and spatio-temporal data mining from mobility data generated by wireless networks, mobile technologies and ubiquitous computing.

Fosca Giannotti
Institute of Information Science and Technologies (ISTI), It
fosca.giannotti@isti.cnr.it

IP6
The Mathematics of Adaptive Execution

Algorithmic execution of large transactions in equity and other markets is a large and growing business. The goal is to optimize the overall execution results relative to some benchmark specified by the client, generally involving some combination of minimum market impact and exposure to volatilty risk. An increasingly important trend in recent years is dynamically adaptive algorithms, that adjust execution in response to short-term variations in estimated market liquidity and volatility. The mathematical challenge is to combine that instantaneous response with a more strategic point of view that optimizes an overall combination of impact cost and volatility risk. We summarize some recent work using dynamic programming to calculate and implement optimally adaptive strategies.

Robert Almgren
Courant Institute of Mathematical Sciences, New York Univers
and Quantitative Brokers
almgren@cims.nyu.edu

CP1
The Development of Generic Formulations Using Artificial Neural Networks and Genetic Algorithms

The Development of Generic Formulations using Artificial Neural Networks and Genetic Algorithms Professor Mike Burton, Mathematics Department, Rhodes University, South Africa, Dr Gareth Witten, Department of Statistical Sciences, University of Cape Town, South Africa Artificial neural networks are universal approximators in the sense that they can be used to approximate any continuous function to an arbitrary degree of accuracy. Since the relationship between a formulation and the corresponding release profile is governed by some continuous function, it follows that a neural network exists which can simulate the chemical process which releases the active ingredient from a drug delivery system. The process of constructing such a neural network will be discussed. Furthermore, it will be shown how the neural network can be deployed in a fitness function for a genetic algorithm. Then it will be shown how a genetic algorithm can be used to discover a formulation for a generic form.

Mike Burton
Department of Mathematics, Rhodes University
m.burton@ru.ac.za

Gareth Q. Witten
Department of Statistical Sciences
University of Cape Town
Gareth@santafe.edu

CP1
Stress Response Gene Regulatory Networks: Mathematical Models Based on Experimental Observations

In multicellular organisms, the defensive cellular responses evoked by environmental stresses involve several interlinked genetic pathways, making it difficult to predict the biological effects of multiple stressors acting together. However, this situation is normal for industrial pollution of soil or water, where several contaminants are usually present together. Based on our experimental observations in Britain and India, we propose and analyze some mathematical models of stress-responsive gene regulatory networks involving significant numbers of genes.

Mainul Haque
University of Nottingham, UK
pmxmh1@nottingham.ac.uk

John King
University of Nottingham
School of Mathematical Science
john.king@nottingham.ac.uk

Matthew Loose, David Pomerai
University of Nottingham, UK
matt.loose@nottingham.ac.uk,
david.depomerai@nottingham.ac.uk

CP1
A Hybrid Model of Interaction Between Tumor Cells and Microenviroment

Fibroblasts and myofibroblasts near the tumor microenvironment are important players in tumor growth and metastasis because of their unique ability to coordinate events which increase cell proliferation especially in breast cancer. It has been experimentally shown that fibroblasts play an important role in promoting tumor growth (Ostrowski Lab, OSU). Our study illustrated tumor cells are able to communicate with stroma through growth factors. A multiscale model of this interaction between stroma and transformed epithelial cells will be presented.

Yangjin Kim
OSU
ykim@mbi.osu.edu

Avner Friedman
Department of Mathematics
The Ohio State University
afriedman@math.ohio-state.edu

Julie Wallace, Ful Li, Ostrowk Ostrowki
The Comprehensive Cancer Center
Ohio State University

julie.wallace@osumc.edu, fu.li@osumc.edu, michael.ostrowski@osumc.edu

CP1

Applying Regular Perturbation Analysis to HCV Viral Load Equations

There are many mathematical models of the evolution of hepatitis type C viral (HCV) load found in the literature. Although viral load evolution is quite complex, there are many successful models able to explain many different evolution paths. New treatments of HCV quickly drive viral loads below detectable limits, called the level of quantitation, giving few data points for researchers to fit. Using regular perturbation methodology we derive and test a series of approximations to a standard model in order to understand tradeoffs between model complexity (number of parameters) and model accuracy.

Jeffrey Saltzman
Merck and Company, Inc.
jeffrey_saltzman@merck.com

CP1

Correction of Regional Propagation Artifacts in Ultrasound Images

Spatial variations of attenuation across tissue layers can result in shadowing and enhancement in ultrasound B-scan images. These artifacts affect the underlying signal backscatter which is the main component of ultrasound images and has clinical significance in detecting diseases and tumors. We present a Backscatter-Contour-Attenuation (BCA) joint estimation model for scatter attenuation compensation in pulse-echo imaging using a set of self-consistent partial differential equations and a contour evolution model. A three-step alternating minimization procedure is adopted to compute the numerical solutions.

Jue Wang
Union College
wangj@union.edu

Yongjian Yu
InfiMed Inc.
yuy@infimed.com

CP1

Modeling Chlamydomonas: A Computational and Mechanical Study

Cell and flagella motilities of microorganisms have been the attractive topics for researchers for many years. As an outstanding model microorganism, Chlamydomonas, a tiny unicellular alga with two hair-like flagella for propelling the cell body through its fluid environment, has been intensively used for the study of numerous fundamental biological processes in cell and molecular biology, cilia-pathology in the human health. However the mechanism governing the motilities of the bi-flagellar is still not well understood. We present a computational fluid-dynamical model that examines variety of the bi-flagellar motilities of Chlamydomonas. This model couples the fluid dynamics governed by Navier-Stokes equations and the internal force generation mechanism by ATP-induced molecular motor proteins.

Xingzhou Yang
Mississippi State University
xyang@math.msstate.edu

Lisa Fauci
Tulane University
fauci@tulane.edu

CP2

Non-Linear Darcy's Equation and Fluid Filtration in Porous Media

We consider non-linear flows in porous media for slightly compressible fluids. A class of non-linear momentum equations is introduced. It covers the three empirical Forchheimer's laws which are widely used by engineers to capture the non-linear characteristics of the flow neglected by Darcy's law. The focus of this work is the stability analysis and long time dynamics of the flows subjected to particular boundary conditions. Theoretical studies are supported by numerical simulations.

Lidia Bloshanskaya
Texas Tech University
Department of Mathematics and Statistics
lidia.bloshanskaya@ttu.edu

Eugenio Aulisa
Department of Mathematics and Statistics.
Texas Tech University
eugenio.aulisa@ttu.edu

Luan Hoang
Texas Tech University
Department of Mathematics and Statistics
luan.hoang@ttu.edu

Akif Ibragimov
Department of Mathematics and Statistics.
Texas Tech University
akif.ibraguimov@ttu.edu

CP2

Tunnel - Aquifer State Function and Flow Integrals

An integral representation of the state function of a semi-infinte aquifer that is drained by a circular tunnel is used to deduce an excat analytic solution. A set of simple and double integrals, which integrands are products of modified Bessel functions of the 2nd kind and trigonometric functions is generated. Another set of integrals, the flow integrals, containing the gradient of the state function is generated when determining the flow induced by the tunnel. Both sets of integrals are computed exactly and expressed in closed forms. Although the analytic solution is not a compact equation it can be truncated retaining its first term which gives an indication on the relation that binds tunnel and soil parameters and can be used for a first evaluation of the water inflow and pressure for engineering practice.

Mohamed El Tani
Lombardi Eng. Ltd.
mohamed.eltani@lombardi.ch

CP2

Optimizing a Mass Consistent Wind Model for a Complex Tropical Island Terrain

The quality of wind fields generated by a mass-consistent wind model over the complex terrain of Sri Lanka was evaluated. Sri Lanka is a tropical island (400 km x 250 km) with high mountains (2,500 m) which is subject to monsoonal wind fields. We tuned the ATHIN mass-consistent model using a synthetic three-dimensional Gaussian mountain profile under geostrophic wind fields as experienced in Sri Lanka to assess parameters such as atmospheric stability, transmissivity and thresholds for residuals that result in simulations that approximate what we expected from analytical solutions. Thereafter, we used these parameters, to simulate monthly climatological wind fields over the Sri Lankan topography. Overall, realistic results were obtained for both strong and weak monsoon periods. The model predicts wind patterns, which are generally consistent with wind climatologies based on surface measurements and with upper air measurements in four stations. The results compare well with available observations. The model simulations are not entirely accurate for coastal areas as the methodology does not incorporate the sea-breeze and mountain breezes. There were some discrepancies in the simulated wind speeds on the lee-side of the mountains. With these limitations, the model is nonetheless useful as a means of obtaining high-resolution wind climatologies for the lower atmosphere. The wind fields obtained shall be useful for wind energy resource estimation, pollution modeling, structural design, water resource assessments and ecological studies.

Ajith Gunaratne
Florida A & M University
Department of Mathematics
ajith.gunaratne@famu.edu

Lareef Zubair
International Research Institute for Climate and Society
The Earth Institute at Columbia
lareef@iri.columbia.edu

CP2

Numerical Approximations of Riemann Solutions to Multiphase Flows Used in Petroleum Engineering

We study two one-dimensional systems of hyperbolic conservation laws that are used to model the multiphase flow in the process of secondary oil recovery. We compute approximate solutions for several examples using a spacetime discontinuous Galerkin (SDG) method based on causal spacetime triangulations and a piecewise constant Galerkin basis. Even though convergence of the SDG method was shown only in the case of strictly hyperbolic genuinely nonlinear Temple class systems, numerical solutions presented in this paper show that the SDG method could be effectively used for approximating solutions to more general problems.

Katarina Jegdic
University of Houston-Downtown
JegdicK@uhd.edu

CP2

Numerical Resolution of Co2 Transport Dynamics

We consider a hyperbolic system of conservation laws describing multicomponent flows through a transport pipeline, with applications to CO2 transport and storage. We demonstrate that numerical dissipation easily leads to an underestimation of the amplitude of pressure pulses and the resulting pipe strain. We argue that recently developed high-resolution methods, particularly adapted to our current model, are essential tools for an accurate operations analysis.

Alexandre Morin, Peder Kristian Aursand, Tore Flåtten, Svend Tollak Munkejord
SINTEF Energy Research
alexandre.morin@sintef.no, pederka@stud.ntnu.no, flatten@math.uio.no, stm@pvv.org

CP2

Implementation of Channel-Routing Routines in the Water Erosion Prediction Project (WEPP) Model

The Water Erosion Prediction Project (WEPP) model is a process-based, continuous-simulation, watershed hydrology and erosion model. It is an important tool for water erosion simulation owing to its unique functionality for representing diverse landuse and management conditions. Its applicability is limited to relatively small watersheds since its current version does not simulate permanent channel flow. In this study we developed a channel-routing module to simulate water flow in a channel network. The module can utilize two methods: numerical kinematic-wave method and Muskingum-Cunge method. Results showed that, for appropriate temporal and spatial discretizations, both numerical solutions compared well with analytical solution of kinematic wave equations for simplified cases; otherwise, numerical dissipation from kinematic wave solution, and numerical dispersion from Muskingum-Cunge solution would occur.

Li Wang, Joan Wu, Sergey Lapin
Washington State University
liwang@wsu.edu, jwu@wsu.edu, slapin@wsu.edu

Fritz Fiedler
University of Idaho
fritz@uidaho.edu

William Elliot
US Forest Service
welliot@fs.fed.us

CP3

Numerical Simulation of the Laser Beam Cutting of Metal Sheet

The numerical simulation of the cutting of metal sheet by a laser beam is a great challenge. The melt front is a free boundary. We simulate this process with the black-box solver FDEM (Finite Difference Element Method). During this solution process we have to stabilize the melt front numerically by a polynomial. FDEM is fully parallelized software for the numerical solution of nonlinear systems of elliptic and parabolic PDEs with the unprecedented feature of an error estimate.

Torsten Adolph, Willi Schoenauer
Forschungszentrum Karlsruhe
Steinbuch Centre for Computing
adolph@kit.edu, willi.schoenauer@iwr.fzk.de

CP3

Analysis of the Growth Kinetics of Boride Layers in Steels

Boriding is the surface boron saturation of metals and alloys with the purpose of increasing their hardness, wear and corrosion resistance in engineering components where their industrial application requires those properties. If the kinetics parameters were known, it would be possible to automate and optimize the boriding process. We present a mathematical model to describe the growth evolution of the boride layers as a function of temperature and surface boron concentration.

Maria Y. Jimenez
Instituto Politecnico Nacional
maria.jimenez.reyes@gmail.com

CP3

The Effect of Vibration on Flow Rate of Non-Newtonian Flow

Non-Newtonian flows appear in a number of industrial applications such as oil production and production of polymers, pharmaceuticals and food products. It has been observed in the field and shown experimentally that vibrational motion induced by acoustic stimulation affects the mean flow rate of non-Newtonian fluids. In present work we propose a mathematical model of unsteady bi-viscous and Bingham fluid flow in two-dimensional cross section of a channel. Proposed model is used to investigate numerically the effect of acoustic wave applied to the flow driven by pressure gradient. It is found that under favorable conditions, the mean flow rate can be significantly increased by acoustic stimulation. Results of numerical simulations for a broad range of vibration amplitudes, frequencies and fluid viscosity will be presented and discussed.

Sergey Lapin
Washington State University
slapin@wsu.edu

Konstantin Matveev, Mohsen Asle Zaeem
Washington State University
School of Mechanical and Materials Engineering
matveev@wsu.edu, mohsen.a.zaeem@gmail.com

CP3

Modelling and Optimization of Ship Hull Geometries

This work relates to the numerical optimization of shape geometries. We consider ship hull geometries for ships with the Voith-Schneider® Propeller (VSP), an efficient propulsion and steering device. The consideration of the VSP introduces the need for different geometric models than for ships with conventional scrub propellers. In this talk, we discuss the parametrization and the numerical optimization, where we use Computational Fluid Dynamics (CFD). This is joined work with Voith funded by the BMWi (Federal Ministry of Economics and Technology,Germany).

Juan C. Matutat, Michael Hopfensitz, Karsten Urban
Institute of Numerical Mathematics, University of Ulm
juan.matutat@uni-ulm.de, michael.hopfensitz@uni-ulm.de, karsten.urban@uni-ulm.de

CP3

Finite Approximations for Some Discrete Convolutions

As a rule all applied problems are described by boundary value problems for partial differential equations, and(or) by integral equations. Very often the integral operator mentioned is a convolution operator in a certain generalized sense. The computer can't speak to continual convolution, and it is impossible to speak to discrete but infinite convolution ones too. Then the problem is arised on a change of discrete convolution by finite object which is convenient for a computer, and which is conserving all properties of continual convolution as much as possible. One suggests a certain approximation variant for a class of singular discrete convolutions.

Vladimir B. Vasilyev
Department of Mathematics and Information Technologies
Bryansk State University
vbv57@inbox.ru

CP3

Efficient Calculation of Fluid Structure Interaction in Ship Vibration

The hydrodynamic mass effect of the surrounding water must be included in realistic simulations of global ship vibration. The effect of water modeled by the hydrodynamic added mass matrix allows for the simulation of ship vibrations up to approximately 25 Hz. In this presentation approaches for extending ship vibration analysis into higher frequency ranges based on reduction methods for the hydrodynamic mass matrix and making use of fast solution methods for the exterior fluid problem are discussed.

Heinrich Voss
Hamburg Univ of Technology
Institute of Numerical Simulation
voss@tu-harburg.de

Alexander Menk
Robert Bosch GmbH, Stuttgart
alexander.menk@gmx.net

Marc Wilken, Christian Cabos
Germanischer Lloyd, Hamburg
marc.wilken@gl-group.com, christian.cabos@gl-group.com

CP4

Molecular Dynamics Simulation of Liquid Methyl Chloride with a Treecode Ewald Summation Method

We will present results on the application of the treecode method to the computation ofthe real space part of the Ewald sum in molecular dynamics simulation. We show that for reasonable parameters, the treecode speeds up the Ewald sum for large systems and reproduces the structural and dynamical properties of the liquid within error bars.

Henry A. Boateng
Department of Mathematics
University of Michigan
boateng@umich.edu

Robert Krasny
University of Michigan

Department of Mathematics
krasny@umich.edu

Eitan Geva
University of Michigan
department of chemistry

CP4

Uncertainty Quantification for Radioactive Waste Disposal

Motivated by concerns about greenhouse gas emissions, nuclear power is once again finding favour as a low-carbon technology for electricity generation. However, the problem of long-term disposal of radioactive wastes produced by a nuclear power programme has still to be satisfactorily resolved. A major scientific challenge is the characterisation and quantification of uncertainties inherent in respository performance assessments. Recent advances in uncertainty quantification and their application to radioactive waste disposal will be presented.

K. Andrew Cliffe
University of Nottingham
andrew.cliffe@nottingham.ac.uk

CP4

Large-Scale Probability Density Evolution Using Ensemble Kalman Filter

Recently Ensemble Kalman Filters (EnKF) have gained increasing popularity for history matching and continuous reservoir model updating. It solves the underlying *Ito* stochastic problem and the probability density evolves due to three components: deterministic drift due to object dynamics, diffusion due to the random component, and reactive reinforcement due to measurements. I explore some critical issues related with the use of EnKF for history matching a large oilfield with substantial production history. These include streamline-based covariance localization and optimal initial member selection.

Ajitabh Kumar
Chevron Corp, San Ramon
ajitabh.kumar@gmail.com

CP4

Free Transverse Vibrations of Nonhomogeneous Orthotropic Rectangular Plates of Linearly Varying Thickness

Effect of nonhomogeneity together with the thickness variation on the vibrational characteristics of orthotropic rectangular plates has been analyzed on the basis of classical plate theory. Nonhomogeneity of the plate material is assumed to arise due to the linear variations in Youngs moduli in the respective directions and density along both the directions of the orthotropy. Rayleigh-Ritz method with boundary haracteristic orthogonal polynomials in two directions has been used in this study. These polynomials satisfying geometric boundary conditions are generated using the Gram-Schmidt process.

Roshan Lal, Yajuvindra Kumar
Indian Institute of Technology Roorkee
rlatmfma@iitr.ernet.in, yaju_saini@yahoo.com

CP4

The Machine Interference Model in a Flexible Manufacturing System: A Stochastic Approach

In this proposal, we modeled a line of production in a system of flexible manufacture (MFS) using stochastic differential equations, Markov chains and a generalized Poisson process in order to obtain indicators of its operation efficiency. We used the approach of the interference model to obtain some formulas to compute the steady-state performance measures including the interference loss and some limiting distributions. The theoretical and simulation results are reported and practical applications are suggested.

Gilberto Pérez-Lechuga
Advanced Research Center on Industrial Engineering
Hidalgo State University
glechuga2004@hotmail.com

A.A. Karelyn
Advanced Research Center on Industrial Engineering
Hidalgo State University, Mexico.
skarelin@uaeh.readuaeh.mx

M.G. Munoz-Oran
Department of Computer Science
University Center 21st Century, Mexico
morayma76@hotmail.com

E. S. Hernandez-Gress
Advanced Research Center on Industrial Engineering
Hidalgo State University, Mexico
evah@uaeh.edu.mx

CP4

A High Order Numerical Method for Computing Physical Observables in the Semiclassical Limit of the One Dimensional Linear Schrödinger Equation with Discontinuous Potentials

We develop a fourth order numerical method for the computation of multivalued physical observables in the semiclassical limit of the one dimensional linear Schrödinger equation with discontinuous potentials. The method consists of high order methods for solving the classical Liouville equation with discontinuous potentials and evaluating one dimensional delta function integrals with discontinuous kernel functions. Numerical examples are presented to verify the high order accuracy of our method.

Xin Wen
Institute of Computational Mathematics
Chinese Academy of Sciences
wenxin@amss.ac.cn

CP5

Generating Fabrication-Ready Structures from Constitutive Equations

Constitutive equations of structural unit trusses and unit cells allow for the generation of fabrication-ready three-dimensional models of lattice structures for use in component designs. The local magnitude of the structural loading determines the type, orientation and sizing of the unit truss/cell. There are five types of unit trusses/cells of varying complexity to draw from, including two proprietary types. The comparative performance metrics of these two

will be included.

Douglas L. Cook, Douglas Stahl, Ph.D., Brad Knier
Milwaukee School of Engineering
cookd@msoe.edu, stahl@msoe.edu, knierb@msoe.edu

CP5

Volume Estimation of Molded Artifacts by B-Splines

We consider the problem of estimating the volume of a closed non-metallic semi-spherical surface formed by a molding process. A coordinate measuring machine was used to probe the surface and produce a scattered set 0f (x,y,z) data points on the surface. Based upon earlier work in the literature a B-spline model of the surface was developed through a least squares fit to the data. Once developed the model was used to estimate the volume by integration. An application to simulated lung cance nodules will be given.

David E. Gilsinn
Mathematical and Computational Sciences Division
National Institute of Standards and Technology
dgilsinn@nist.gov

CP5

Mesh Generation for Ship Hull Geometries for Optimization

This work relates to the numerical optimization of shape geometries. In this talk, we focus on the mesh generation that is required for the shape optimization of ship hull geometries for ships with Voith-Schneider-Propeller (VSP). We start by a predominant hexahedral mesh for such geometries. Besides an automatic and parametric meshing program was implemeted. To meet the requirements for the mesh, meshing methods were developed. This is joined work with Voith funded by the BMWi.

Michael Hopfensitz, Juan C. Matutat, Karsten Urban
Institute of Numerical Mathematics, University of Ulm
michael.hopfensitz@uni-ulm.de,
juan.matutat@uni-ulm.de, karsten.urban@uni-ulm.de

CP5

Geometry from Markup: Virtual Model Creation Using Semantic Markers

Creating virtual content is cumbersome and time consuming. FXPAL has developed a novel approach to creating virtual models from images by first marking up rooms or objects with physical markers that have associated meanings. A number of elegant and simple-to-state problems arise concerning under what conditions the geometry can be reconstructed from the marker positions, orientations, and associated semantic information. We describe results and counterexamples, and list open problems.

Eleanor Rieffel, Don Kimber, Jim Vaughan
FXPAL
rieffel@fxpal.com, kimber@fxpal.com, jimv@fxpal.com

CP6

Markov Chain Modeling of Time Series

Our goal is to derive simple, finite state Markov models that describe key features of real-valued time series data. We give a method for fitting a Markov chain of optimal order to the data, using maximum likelihood estimation combined with cross-validation. We apply our method to real financial data, where we can (in)validate assumptions made in options pricing models. We also present extensive results with synthetic data, showing the method's validity.

Harish S. Bhat, Nitesh Kumar
University of California, Merced
Applied Mathematics
hbhat@ucmerced.edu, knitesh@gmail.com

CP6

Sensitivity of Option Pricing to Errors in the Parameters of the Underlying Stochastic Dynamics

Robust pricing of options on financial assets requires good parametric estimates of underlying stochastic models. Here we compute bounds on the sensitivity of option prices to errors on the parameters of Heston's joint SDE model for asset price and volatility. We implement an efficient numerical scheme to solve the PDEs satisfied by the derivatives of the option price with respect to the model parameters. We then combine these sensitivity estimates with the theoretical estimates of parametric errors which we had earlier derived for the joint SDE Heston model. We outline concrete numerical results on error sizes for the pricing of European options based on S&P 500 index data.

Robert Azencott
Department of Mathematics
University of Houston
razencot@math.uh.edu

Yutheeka Gadhyan, Roland Glowinski
University of Houston
yutheeka@math.uh.edu, roland@math.uh.edu

CP6

A Revenue Maximizing Strategy Based on Bayesian Analysis of Demand Dynamics

This talk presents a revenue optimization approach with demand learning and dynamic pricing for firms in an oligopoly service network. We introduce a state-space revenue management model, which incorporates evolutionary demand dynamics and a nonparametric model describing the evolution of price sensitivities. We develop a Markov chain Monte Carlo (MCMC) method to estimate state variables, parameters, and coefficient functions such that future price sensitivities can be predicted. Based on this prediction, optimal pricing policy for the next planning period is obtained by simulated annealing algorithm. Simulated data example shows that our new method is efficient and robust for integrating demand learning and dynamic pricing.

Jiahan Li
Department of Statistics
Pennsylvania State university
jiahanli@psu.edu

Tao Yao
Department of Industrial and Manufacturing Engineering
Pennsylvania State University
taoyao@psu.edu

Haibing Gao
Department of Statistics

University of Florida
haibing@stat.ufl.edu

CP6

Gradient Boosting for Joint Regression Modeling of Mean and Dispersion with Insurance Applications

We consider the joint regression of the mean and dispersion for a conditional response distribution from the exponential dispersion family. The focus in this paper is on the Normal, Gamma and Inverse Gaussian distributions, which are continuous distributions from the exponential dispersion family for which the likelihood takes a particular simple form. The regression methodology is based on Gradient Boosting (Friedman, 2001) with extensions to incorporate dispersion modeling. The proposed approach offers certain advantages over Generalized Linear Models, including for example, the easy incorporation of relevant nonlinear and low-order co-variate interaction effects in the regression function; robust and computationally-efficient modeling procedures suitable for large, high-dimensional data sets; and the ability to use high-cardinality categorical co-variates directly in the regression without any *ad hoc* pre-processing or grouping of the feature levels that is often required in other modeling procedures for computational tractability. We provide the motivation, background theory and algorithmic details of the proposed methodology along with some illustrative computational examples from actuarial applications.

Ramesh Natarajan
IBM Thomas J. Watson Research Center
nramesh@us.ibm.com

CP7

Modeling of Rapid Shear in High-Speed Machining

A high-speed machining operation provides an interesting setting for the study of plastic flow under extreme conditions. In the thin primary shear region where cutting takes place, it is not uncommon to have strains on the order of 1-10, strain rates on the order of 104-105 s-1, and an increase in temperature on the order of a millisecond from ambient to a significant fraction of the melting temperature, corresponding to a heating rate on the order of 106 C s-1. Recent experimental results and attempts to model them from the point of view of nonlinear dynamics will be discussed.

Tim Burns
NIST
Mathematical and Computational Sciences Division
burns@cam.nist.gov

CP7

Stimulation and Optimization Problems of Some Technological Processes in Microelectronics

Some simulation and optimization problems of VLSI production technological processes i.e. of ion-simulation diffusion are considered. For each process the L.S. Pontrygin maximum principle has been proved and the numerical solution method based on this principle has been developed. Proposed solution has lesser systematic errors and future perspectives higher reliability. Brought are the results of mathematical modeling and experiments, along with the calculation technique. The results substantiating the method efficiency are presented.

Valery E. Grishin
Russian State Aviation Technology
Jefunr@hotmail.com

Leonid A. Muravey
Russian State Aviation Technology University
godendm@mail.ru

CP7

Applications of Delayed Optimal Control Problems

We consider optimal control problems with delays in control and state variables. The delayed (retarded) control process is subject to control and state constraints. Necessary optimality conditions are given in form of a Pontryagin type Minimum Principle. Using suitable discretization schemes, the optimal control problem is transcribed into a large-scale optimization problem which can be solved by Interior-Point or SQP methods. The main focus in this talk is on two practical applications: (1) optimal control of a continuous stirred tank reactor (CSTR); (2) optimal control in a model for oil-exploration. Joint work with Laurenz Göllmann, Daniela Kern and Willi Semmler is gratefully acknowledged.

Helmut Maurer
Universität Münster
Institut für Numerische und Angewandte Mathematik
maurer@math.uni-muenster.de

CP7

Measurement of System Resilience: Application to Chemical Supply Chains

Within the context of infrastructure and economic systems analysis, the authors define resilience as follows: given the occurrence of a particular, disruptive event, the resilience of a system to that event is its ability to efficiently reduce both the magnitude and duration of the deviation from desired system performance levels. We propose a new methodology, originating from optimal control applications, for measuring system resilience. The approach is demonstrated through applications to chemical supply chains.

Eric D. Vugrin
Sandia National Laboratories
edvugri@sandia.gov

R. Chris Camphouse
Sandia National Laboratories
Carlsbad Programs Group
rccamph@sandia.gov

P. Downes, Mark Ehlen, Drake Warren
Sandia National Laboratories
psdowne@sandia.gov, maehlen@sandia.gov, dewarre@sandia.gov

CP8

Finite Element Solution to Double Diffusion Transport Phenomena to Stretching Sheet

In numerous industrial transport processes, convective heat and mass transfer takes place simultaneously. Phenomena involving stretching sheets feature widely in for example, production metal casting. In such processes metals or alloys are heated until molten, poured into a mould or die, and liquid metal is subsequently stretched to achieve the desired product. When the super heated melt issues from the dies it loses heat and contract as it cools, a stage in metallurgical processing referred to as liquid state contraction. The mechanical properties of the final product depend to a great extent on the heat and mass transfer phenomena, the cooling rate, surface mass transfer rate etc. Some other important industrial applications of stretching sheet transport phenomena are the extrusion of a polymeric sheet from a die or the drawing of plastic films. The purpose of the present investigation is therefore to study the coupled fluid flow, heat and mass transfer phenomena over a stretching sheet with nonlinear velocity, for micropolar fluids. Such a study has not been reported earlier in the literature and is important is materials processing.

Rama Bhargava
Indian Institute of Technology Roorkee
bhargava_iitr@rediffmail.com

CP8

Topological Analysis for Computation of Ray/surface Intersections

Many graphics and animation applications depend upon convergence of geometric algorithms. The use of topological analysis is shown to improve geometric convergence in graphics applications using ray-tracing. An algorithm is presented that extends ray-tracing over a richer family of input surfaces and numerical examples are given.

Justin P. Bisceglio
Blue Sky Studios
University of Connecticut, Department of Computer Science
justin.bisceglio@gmail.com

Thomas J. Peters
University of Connecticut
tpeters@engr.uconn.edu

CP8

Matrix Network Models for Industrial Systems

We represent a new methodology for modelling industrial systems and processes. It is founded on the method of multidimensional matrix networks and multidimensional matrix representations of industrial functions and industrial operations. A matrix network is, by definition, a collection of multidimensional matrices (vertices representing industrial units) interconnected by another matrix collection (nodes representing ties between units).In this context, each unit can be represented by its own matrix network model. This allows matrix network modelling to be functional and multilevel.

Armenak S. Gasparyan
Program Systems Institute of RAS
armen@armen.pereslavl.ru

CP8

Immersed Boundary Modeling and Simulation for Concentrated Suspensions

One major example of dense multiphase flows in engineering is the extrusion process which is a crucial part in the industrial production of ceramic products. We study the extrusion batch flow through multi-scale modeling and a modified immersed boundary (IB) method with direct-forcing. A software package (IBAMR) with support for Cartesian grid adaptive mesh refinement developed by B. Griffith from New York University is utilized to implement the IB method. A series of numerical experiments for suspensions with mono-disperse and poly-disperse particles provide evidence for the different roles of particle characteristics and fluid properties in determining the rheology and microstructure of the suspension.

Weigang Zhong
Corning, Inc.
zhongwg@corning.com

MS1

Numerical Simulation of Turbulent Hydrogen Combustion

There is little work in the literature that deals with premixed flames in the distributed burning regime (or broken reaction zone). Based on a series of papers by Mansour and Chen, which looked at highly-stretched premixed methane Bunsen flames, Peters (2000) concludes that a premixed flame is unable to survive in the broken reaction zone. Single vortex-flame interactions were considered experimentally by Roberts et al. (1993) and numerically in two dimensions by Poinsot et al (2006). In both cases, a quenching zone was identified. Further details can be found in Peters (2000) and Poinsot and Veynate (2005). A recent study in supernova flames (Aspden et al 2008) found that quenching was not observed even at a Karlovitz number of 230 and moreover the flame speed was enhanced by the turbulence. This high Karlovitz number flame presented very different burning to the lower Karlovitz number flames. Mixing was dominated by turbulence a distributed flame was observed. The present study considers three dimensional simulations of lean premixed hydrogen flames in a turbulent background. The Karlovitz number is varied from 10 to 1560, and a range of equivalence ratios are considered. Under the conditions studied, quenching was not observed, even at Ka=1560. It was found that the low equivalence ratio did not transition to a distributed flame at Ka=1560, but it was found to be possible at the higher equivalence ratio. Diffusion processes are examined to demonstrate the importance of turbulent mixing.

Andrew Aspden
LBNL
AJAspden@lbl.gov

MS1

Adaptive Mesh Refinement for Reacting Flow in Porous Media

Abstract not available at time of publication.

John B. Bell
CCSE
Lawrence Berkeley Laboratory
jbbell@lbl.gov

MS1

Hybrid Algorithms for Simulation of Fluids at the Microscale

We consider hybrid algorithms based on an adaptive mesh refinement framework in which a particle algorithm is em-

bedded at the finest grid of the mesh hierarchy. Here, we focus on hybridization of a direct simulation Monte Carlo algorithm combined with the compressible Navier Stokes equations. At the continuum level we consider both a deterministic Navier Stokes solver and a modified solver based on the stochastic Landau-Lifshitz-Navier-Stokes equations. We will discuss the impact of fluctuations on the dynamics and demonstrate the necessity to include a stochastic forcing term at the continuum level to accurately model microscopic behavior.

Alejandro Garcia
Lawrence Livermore National Laboratory
San Jose State University
algarcia@algarcia.org

MS1

A Reduced Basis Model for Nano-mosfet Simulation

As size of electronic devices shrinks to nanometer scale, quantum effects become increasingly important in describing charge transport phenomenon in these devices. However, simulation of quantum effects, which involves self-consistently solving a coupled Schrodinger-Poisson system of equations, is usually computationally intensive. In addition, nanoscale devices, such as nano-MOSFET, nanowires and nanotubes, must be optimized to maximize performance; this is only feasible if one can efficiently explore the design parameter space. New modeling and simulation capabilities can thus greatly facilitate design of nanoscale devices. Although a wide range of numerical schemes have been proposed for nanoscale device modeling, most require solving a large nonlinear system of algebraic equations repetitively. While very detailed solution can be obtained, the large computational cost severely limits the potential of simulation to speed up design and optimization of nanoscale devices. Here, we couple the reduced basis method with the subband decomposition method to achieve significant improvement in the overall efficiency of the simulation. By exploiting a posteriori error estimation procedure and greedy sampling algorithm, we are able to design an algorithm where the computational cost is reduced significantly. In addition, the computational cost only grows marginally with the number of grid points in the confined direction.

George Pau
LBNL
GPau@lbl.gov

MS2

Applications of Statistical Data Modeling and Analysis at Boeing

Statistical data fitting methodologies that have proven useful for modeling a variety of phenomena of interest within Boeing and to some extent the broader industry will be discussed. The primary methodologies considered will be multiple adaptive regression splines, projection pursuit regression, and support vector machines aka radial basis functions. Most of the applications arose from work done at Boeing though some comments will be made regarding applications outside Boeing. Most of the problems considered are regression problems where the desire is to predict quantitative outputs as opposed to classification which predicts qualitative outputs.

David Clark
The Boeing Math Group
david.m.clark@boeing.com

MS2

Nonlinear Schemes for Multivariate Splines

We will discuss a few of the many applications of nonlinear optimization techniques for data fitting with tensor product splines. Among the capabilities this approach affords are robust handling of underdetermined overdetermined systems and shape control. The specific applications will come the airplane industry.

Thomas A. Hogan
The Boeing Math Group
thomas.a.hogan@boeing.com

MS2

Calibrating Agent Based Models to Real World Data

Agent based models are powerful tools for modeling processes from the ground up. Usually parameters are introduced into the model that need to be modified or calibrated to ensure the model accurately fits real world data. Adaptive techniques are described here which reduce the correlation of model errors against the data drivers in the model. Specific examples will be shown from econometric models based on virtual populations.

Steve Noble
VP, Software Development
DecisionPower, Inc
steve@noblerwe.org

MS2

Ensembles of Decision Trees – a Rich Vein for Data Mining

Taiga is a sophisticated tool that uses Ensembles of Decision Trees and is capable of producing accurate diagnostic and prognostic models on supervised and unsupervised problems for feature-set reduction, classification, regression, clustering, and anomaly detection. Innovations include: automatic intelligent data imports; optimized data representations that enable handling of massive datasets; genetic methods for tree growing that use Pareto techniques for multi-objective learning; methods for transforming trees into Hilbert Space analysis and redundancy elimination; and interactive visualization and drill-down capabilities to provide explanations for observed behavior.

John M. Trenkle
Senior Scientist
Michigan Aerospace Corporation
jtrenkle@michiganaerospace.com

MS3

Hightech Meets Handmade - Processing Scanned Archaeological Pottery

Abstract not available at time of publication.

Guido Brunnett
Chemnitz University of Technology
guido.brunnett@informatik.tu-chemnitz.de

MS3

Real-time Triangulation of Point Streams

Hand-held laser scanners are used in industry for reverse engineering and quality measurements. An interactive triangulation of the scanned surface points can assist the human operator. Our method computes a triangulation of the point stream generated by the laser scanner online, i.e., the data points are added to the triangulation as they are received from the scanner. Multiple scanned areas and areas with a higher point density result in a finer mesh and a higher accuracy.

Klaus Denker
TU Kaiserslautern
denker@informatik.uni-kl.de

MS3

Haptic Rendering of Scanned Point Sets Using a Fast, Local Reconstruction

Point sets are the initial data acquired for reverse engineering of real world models. For fast exploration and decision where to spend more points during scanning, algorithms have been developed for rendering point sets graphically. Like for surface models, we present an approach for haptic rendering of point set data, which uses a fast, local surface reconstruction consistent with a spatial nearest neighborhood of a surface point. We show how to resolve cases, where the spatial nearest neighborhood falls apart into several surface parts.

Christoph Fuenfzig
Universite de Valenciennes et du Hainaut-Cambresis
Universite de Bourgogne
Christoph.Fuenfzig@u-bourgogne.fr

MS3

High Resolution, Real-time 3D Scanning

With recent advancements of digital technology, real-time 3D scanning plays an increasingly important role in enormous fields including manufacturing, medical sciences, and entertainment. Over the past few years, real-time 3D scanning technologies have been advancing drastically rapidly. We have successfully developed a system that can achieve 180 fps scanning system with 300K points per frame. In this lecture, I will summarize the most recent advancements, and discuss the challenges to further advance this technology.

Song Zhang
Iowa State University
song@iastate.edu

MS4

Interactions Between Machine, Work-piece, and Process Dynamics in Milling Machines

In this talk a mathematical model will be discussed that characterizes the interaction between machine, work-piece, and process dynamics for a complex milling system. While the machine dynamics is modeled in terms of a standard multi-body system, the work-piece is described as a linear thermo-elastic continuum. The coupling of both parts is realized by an empirical process model permitting an estimate of heat and coupling forces occurring during milling. The governing equations will be described emphasizing the coupling, then an analytical result will be outlined concerning the well-posedness of the system. The presentation is concluded with some numerical results showing the dynamics of this complex thermo-mechanical system.

Dietmar Hoemberg
Weierstrass Institute for Applied Analysis and Stochastics
hoemberg@wias-berlin.de

MS4

Mathematical Models for Simulating Micro Grinding Processes

Micro material removal processes are essentaial for manufacturing components with high surface quality. These processes are mainly used in medical, electronics and automotive industry. A precise mathematical model for micro cutting operations needs to consider the relative motion between tool and workpiece (process-structure intreraction). The process model - in particular - cannot b based on the standard macro force models: micro grinding operates with different speeds and much smaller infeed rate, hence the classical Kienzle or Altintas models for cutting forces or the more complex Malkin model do not apply. Hence we develop a mathematical simulation tool, which is based on an updated force model obtained from experimental micro measurements. The elastic deformation of the work tool in opposite direction to the feed is influenced by the forces during the process occur. The developed model includes the effects of the process kinematics and tool edge serration. Simulation results will be presented for the actual infeed rate and the actual depth of cut as well as for the forces.

Peter Maass
Center for Industrial Mathematics
University of Bremen
pmaass@math.uni-bremen.de

MS4

Optimal Multi-beam Laser Welding by State-constrained Semi-infinite Optimization

A semi-infinite optimization problem with a pointwise and an isoperimetric state constraint serves as a model for the optimization of a three-beam laser welding process for alumnium alloys. Position, size and intensity of the two auxiliary laser beams are the parameters that are to be optimized. The main constraint is given by a quasi-stationary heat equation for the temperature field induced by the laser beams. A major role is played by two state constraints. They either avoid melting under the two auxiliary laser beams or restrict the opening displacement which may be the source of hot cracks. The ultimate aim of the optimization namely is to avoid hot crack initiation. Although necessary conditions can be developed, the complexity of these conditions clearly promote the approach “first discretize than optimize’. Numerical results that have been obtained this way will be presented. Moreover, the optimal solution can be verified experimentally.

Hans Josef Pesch
University of Bayreuth, Germany
Chair of Mathematics in Engineering Sciences
hans-josef.pesch@uni-bayreuth.de

Verena Petzet
Chair of Mathematics in Engineering Sciences
University of Bayreuth
verena.petzet@uni-bayreuth.de

MS4

Adaptive Finite Elements in the Simulation of NC-Shape Grinding

The simulation of the NC-shape grinding process consists of two parts: A geometric-kinematical simulation represents the workpiece and includes a process force model. The spindle and the grinding wheel of the grinding machine are considered in a finite element simulation. Adaptive finite element methods, based on dual weighted error estimation, achieve the desired accuracy at minimal numerical cost. The talk concludes with a discussion of numerical results.

Andreas Rademacher
Institute for Applied Mathematics, Chair
University of Technology Dortmund
Andreas.Rademacher@mathematik.uni-dortmund.de

MS5

High-performance Software for Multiphysics Simulations Using Structured Grids

Abstract not available at time of publication.

Phillip Colella
Lawrence Berkeley National Laboratory
PColella@lbl.gov

MS5

Numerical Simulation of Viscoelastic Fluids

We present the mathematical challenges and implementation details associated with computing incompressible non-Newtonian flows using the Oldroyd-B model for viscoelasticity. Our numerical approach is a conservative finite-difference method using an embedded boundary approach for irregular geometry. Based on our analysis, we are able to augment existing solution methodologies for the incompressible Navier-Stokes equations and compressible fluid dynamics. The resulting algorithm is second-order in space and time, and is able to compute flows from the Newtonian limit to the elastic limit.

Andrew Nonaka
LBNL
AJNonaka@lbl.gov

MS5

CFD Modeling of the San Francisco Bay and Delta

Water resource management in the San Francisco bay and delta requires hydrodynamic simulation over multi-scale domains with complex geometry. Typical study problems involve a simulated time that varies from months to years, which frequently means that simulations are performance bound. To address these requirements, we are developing a mixed 2D-1D hydrodynamic model for a shallow water estuary that is designed for parallel computation on tens to hundreds of processors. Adaptive mesh refinement provides efficient handling of multi-scale problems as well as an infrastructure for linking 1D and 2D calculations. In addition, we have developed a fast grid generation algorithm that uses high-resolution digital elevation maps as well as a particle transport model.

Peter O. Schwartz
Lawrence Berkeley Laboratory
poschwartz@lbl.gov

Eli Ateljevich
California Dept. of Water Resources
eli-sava@pacbell.net

MS5

Numerical Simulation of Polymer Flow in Microfluidic Devices

We present simulation results from a computational model of DNA flow in microfluidic devices. This work is important because computational models, which currently do not exist for these complex multiscale flows, are needed to design miniaturized devices which leverage MEMS technology for many significant applications including pathogen detection as well as continuous monitoring and drug delivery. Our model is based on a fully coupled fluid-particle numerical al- gorithm with both stochastic and deterministic components in a bead-rod polymer representation. We have applied this work to DNA extraction in a microfluidic PCR chamber used in a pathogen detection system.

David Trebotich
LBNL
treb@lbl.gov

MS6

KNIFE: KerNel Iterative Feature Extraction

Selecting important features in non-linear or kernel spaces is a difficult challenge in both classification and regression problems. When many of the features are irrelevant, kernel methods such as the support vector machine and kernel ridge regression often perform poorly. We propose weighting the features within a kernel with a sparse set of weights that are estimated in conjunction with the original classification or regression problem. The iterative algorithm, KNIFE, alternates between finding the coefficients of the original problem and finding the feature weights through kernel linearization. In addition, a slight modification of KNIFE yields an efficient algorithm for finding feature regularization paths, or the paths of each feature's weight. Simulation results demonstrate the utility of KNIFE for both kernel regression and support vector machines with a variety of kernels. Feature path realizations also reveal important non-linear correlations among features that prove useful in determining a subset of significant variables. Results on microarray data are also given.

Genevera I. Allen
Stanford
Dept. of Statistics
giallen@stanford.edu

MS6

Strategic Topology

Solving robotic tasks involves building planners able to deal with uncertainty. This talk shows how combinatorial topology informs that planning process by characterizing the capabilities of robotic systems topologically. Planning problems, particularly for robotic manipulation tasks, may often be cast as discrete graph search problems. Motions in the graph are generally nondeterministic or stochastic as a result of control and sensing errors in the underlying physical system. The global capabilities of such a system may be modeled by the homotopy type of a "strategy complex". The simplices of this complex may be viewed as the eventually-convergent control laws (aka plans or strategies) possible on the graph. One result is a controllability theorem: The robot can move anywhere in the graph despite control uncertainty precisely when the graph's strategy complex is homotopic to a sphere of a certain dimension. The strategy complex resides in a space of motions, but one can compress it back onto the graph, without losing homotopy type. Viewed on the graph, nonsimplices of the simplicial complex have intuitive meaning: they represent potentially inescapable regions of the graph. One can further understand the capabilities of a system via open covers whose open sets are intersections of Euclidean halfspaces determined by the possible motions and their execution times. The nerve of such a cover has the same homotopy type as a time-bounded variant of the strategy complex.

Michael Erdmann
Carnegie Mellon University
Robotics Institute
me@cs.cmu.edu

MS6

Regularization Methods for Collaborative Filtering

We use convex-relaxations to obtain regularized low-rank solutions for large-scale matrix completion problems. With warm-starts we efficiently compute entire regularization path of solutions. The computationally intensive part of the algorithm is computing a low-rank SVD. Exploiting matrix structure this is done linear in matrix dimensions(complexity). Our semidefinite-program is scalable to large matrices: it can fit a rank 60 approximation to the full "Netflix' training set in 9.7 hours.

Rahul Mazumder
PhD student, Dept Of Statistics
Stanford University
rahulm@stanford.edu

Trevor Hastie
Professor, Dept of Statistics; Health Research and Policy
Stanford University
hastie@stanford.edu

Robert Tibshirani
Professor, Dept of Health Research and Policy; Statistics
Stanford University
tibs@stanford.edu

MS6

A Penalized Matrix Decomposition, with Application to Sparse Clustering

We present a penalized matrix decomposition, a new framework for computing a rank K approximation for a matrix. We approximate a $n \times p$ matrix $\mathbf{X}$ as $\sum_k d_k \mathbf{u}_k \mathbf{v}_k^T$, where $\mathbf{u}_k$, d_k, and $\mathbf{v}_k$ minimize the squared Frobenius norm of $\mathbf{X} - \hat{\mathbf{X}}$, subject to constraints on $\mathbf{u}_k$ and $\mathbf{v}_k$. Here, $\mathbf{u}_k$ and $\mathbf{v}_k$ are vectors of lengths n and p, and d_k is a scalar. We show that when this decomposition is applied to a data matrix, it can yield interpretable results. Moreover, when applied to a dissimilarity matrix, this leads to a method for sparse hierarchical clustering, which allows for the clustering of a set of observations using an adaptively-chosen subset of the features. These methods are demonstrated on the Netflix data and on a genomic data set.

Daniela M. Witten
Department of Statistics
Stanford University
dwitten@stanford.edu

Robert Tibshirani
Dept. of Statistics
Stanford University
tibs@stat.stanford.edu

MS7

Observations on Biological Modeling

MSRI has sponsored an ongoing series of symposia on mathematical problems in biology. The problems have ranged from identifying DNA sequences that are predictive of health and disease to signaling networks in cancer and their description and more. Dr. Bryant will share some observations about the problems that are most likely to advance the state of medical and biological modeling. These are not necessarily problems that will be solved easily, but present challenges to the mathematical community for the next decade or more.

Robert Bryant
Mathematical Sciences Research Institute
bryant@msri.org

MS7

Beyond Descriptive Modeling

The pharmaceutical industry is a large consumer of statistics, modeling, simulation and other mathematics. Typical tools and technologies are over 100 years old. These tools have produced little; drug development has slowed dramatically in the last decade and costs have escalated. Biology reflects hierarchical information, e.g., DNA, mRNA, proteins, protein interactions and bio-modules, protein and gene networks, cells, phenotypes, organs, individuals, populations, ecologies, regulatory actions, third-party payers, and shareholder value. Consider electrical engineering. Nobody solves Quantum Electrodynamics or Maxwells Equations when designing a computer. At the lowest level, bulk equations are modified by quantum effects to produce transistors. Transistors are used to build logic circuits. Logic circuits are abstracted into high-level languages that control modules (memory, video, microprocessors, etc.). These approximations in restricted settings. These highly predictive models bear no resemblance to fundamental physics of each process. Medical modeling needs to leap from descriptive models to engineering models.

Bob Korsan
Decisions, Decisions!
BobK@Decide2Act.com

MS7

How to Sequence Interdependent Drug Development Programs

In a portfolio of drugs under development, even if each compound has negative expected value by itself, the portfolio may have a high expected value due to cross-compound learning. We propose an improved method for prioritizing among potential drugs or alternative development programs for a single drug and identify research directions to ensure the method is practical in drug development. Optimal development order can be found by dynamic programming in simplified problems, but we propose and test accuracy of a heuristic method that can account for imperfect learning about multiple attributes (efficacy, safety, etc.), as well as evolving competitive information and constraints.

Kevin Dykstra, Bill Poland
Pharsight Corp.
kdykstra@pharsight.com, bpoland@pharsight.com

MS7

Decision-Making and its Impact on Models

Our movie begins with an academic doing theoretical modeling and basic research. As the camera slowly zooms out, we recognize a pharmaceutical companys various departments: drug discovery and development, regulatory affairs, marketing, distribution, finance, and executive management. As the zoom out continues, we notice partners, shareholders, and bondholders. At the next level, we identify communities of doctors and patients. Finally we see the complexity of health care systems different designs by region and country. The strategic decisions are increasingly dynamic, complex, and uncertain at each higher level. We must choose which one of several viable, creative alternative strategies is best to deal with the many hundreds, or even thousands, of scenarios of the world that might occur as time marches forward. Most people throw their hands up in despair and say, this is impossible; the best that we can do is to develop a satisfactory strategy for the most likely scenario. But an experienced decision analyst would counter by saying, this is very straightforward and doable; using the right people in the right way, we can choose the right course of action that will create the most overall value. We will illustrate how to accomplish this efficiently, effectively, and comprehensively.

Burke Robinson
Burke Robinson, LLC and Stanford
burke@burkerobinson.com

MS8

A Diffuse-interface Approach for Modeling Transport, Diffusion and Adsorption/desorption of Material Quantities on a Deformable Interface

A method is presented to solve two-phase problems involving a material quantity on an interface. The interface can be advected, stretched and change topology, and material can be adsorbed to or desorbed from it. The method is based on the use of a diffuse interface framework, which allows a simple implementation using standard finite-difference or finite-element techniques. Here, finite-difference methods on a block-structured adaptive grid are used, and the resulting equations are solved using a nonlinear multigrid method. Interfacial flow with soluble surfactants is used as an example of the application of the method, and several test cases are presented demonstrating its accuracy and convergence.

John Lowengrub
University of California, Irvine
Department of Mathematics
lowengrb@math.uci.edu

Xiangrong Li
Univ. Cal/Irvine
xli@math.uci.edu

MS8

Efficient and Accurate Numerical Schemes for the Phase-Field Models for Multiphase Complex Fluids

I shall present an energetic variational phase field model for multiphase incompressible flows which leads to a set of coupled nonlinear system consisting a phase equation and the Navier-Stokes equations. We shall pay particular attention to situations with large density ratios as they lead to formidable challenges in both analysis and simulation. I shall present efficient and accurate numerical schemes for solving this coupled nonlinear system, and show ample numerical results (air bubble rising in water, Newtonian bubble rising in a polymeric fluid, defect motion in a liquid crystal flow, etc.) which not only demonstrate the effectiveness of the numerical schemes, but also validate the flexibility and robustness of the phase-field model.

Jie Shen
Department of Mathematics
Purdue University
shen@math.purdue.edu

MS8

A Multicomponent Phase Field Model for Biofilms

Abstract not available at time of publication.

Qi Wang
Florida State University
Department of Mathematics
wang@math.fsu.edu

MS8

Phase Field Modeling of Actomyosin Driven Cell Oscillations

In this talk, we talk about a phase field modeling of actomyosin driven cell oscillations. In this model, we combined the dynamics of actin and myosin with the shape transformations of cell membranes. A uniform phase field formulation is given. And we developed a 3D code for the simulations. This modeling reveals the potential of using phase field methods as an important tool of biologists.

Xiaoqiang Wang
Florida State University
wwang3@fsu.edu

MS8

Energy Stable and Convergent Schemes for the Phase Field Crystal (PFC) and Modified Phase Field Crystal (MPFC) Equations

The PFC and MPFC equations decribe crystals at the atomic scale in space but on diffusive scales in time. The models account for the periodic structure of a crystal lattice through a free energy functional of Swift-Hohenberg type that is minimized by periodic functions. The models naturally incorporate elastic and plastic deformations, multiple crystal orientations and defects and have been used to simulate a wide variety of microstructures. In this talk I describe energy stable and convergent finite difference schemes and their effcient solution using nonlinear multigrid methods. A key point in the numerical analysis is the convex splitting of the functional energy corresponding to the gradient systems. In more detail, the physical energy in both cases can be decomposed into purely convex and concave parts. The convex part is treated implicitly, and the concave part is updated explicitly in the numerical schemes. I will discuss both first- and second-order accurate convex splitting schemes. The proposed schemes are unconditionally stable in terms of the physical energy and unconditionally solvable, which allows for arbitrarily large time step sizes. This property is vital for coarsening studies that require very long time scales.

Steven M. Wise
Mathematics Department
University of Tennessee
swise@math.utk.edu

MS9
Vision-Realistic Rendering

Vision-realistic rendering (VRR) is the computer generation of synthetic images to simulate a subject's vision, by incorporating the characteristics of a particular individuals entire optical system. VRR provides images and videos of simulated vision to enable patient and doctor to see specific visual anomalies of the patient. Potential candiates contemplating surgery could see simulations of their predicted vision and of various possible visual anomalies that could arise from the surgery, such as glare at night.

Brian Barsky
University of California, Berkeley
barsky@cs.berkeley.edu

MS9
GPU-accelerated Algorithmic Responses

For 3D stereoscopic imaging during eye surgery, algorithms are being created for pupil-limbus detection and tracking. A major design challenge is choosing the appropriate synthesis of mathematics to achieve acceptable image quality, fidelity and resolution to assist surgeons. While progress is being made on those issues with traditional sequential algorithms, attention is also being paid to GPU-acceleration techniques for the real-time demands of ongoing surgery.

Igor Borovikov
Kerner Graphics
San Rafael, CA
igor.borovikov@gmail.com

MS9
The Transition from Surgical to Synthetic

The preceding talks discussed current eye imaging problems with solutions in progress. The aim of these surgical systems is to improve vision. Kerner Graphics started with a business focus on the motion picture industry. Some of our research also has applications to real-time visualizations for molecular and engineering simulations, providing a speculative transition to computer generation of synthetic images to simulate a subject's vision. Our interest in video compression has arisen, partially, to support using archived surgeries for education. The mathematics used includes topology, geometry and numerical analysis (as well as whatever is opportunistically appropriate!).

Thomas J. Peters
University of Connecticut
tpeters@engr.uconn.edu

MS9
Image Processing Challenges for Eye Surgery

Having developed a digital platform that eye surgeons, and others, are using for microscopic visualization (in full HD and 3D with minimal latency), TrueVision is now moving on to make full use of the digital capabilities of the system. This includes applications that provide measurements and guidance during surgery. Our paper will present some examples of these procedures and illustrate them with stereo 3D recordings.

Michael Weissman
TrueVision Systems
Santa Barbara, CA
mweissman@truevisionsys.com

Burton Tripathi
TrueVision Systems
btripathi@truevisionsys.com

MS11
A Computational Database for Turbulent Flow

We describe early experiences with a *computational database* for cyber-enabled discovery of spatio-temporal transport and mixing dynamics in simulated geophysical flows. Our database combines the machinery of data retrieval with powerful computational facilities tailored to dynamic representations of irregular time-dependent structures. Our database overcomes the limitations of the relational model by supporting an imperative style of query that conserves spatial locality in numerical algorithms. It is application neutral, and could help transform the discovery process in any field involving complex time-dependent, multi-scale physical phenomena that admits mathematical rules to identify features of interest.

Scott B. Baden, Alden King
Department of Computer Science and Engineering
University of California, San Diego
baden@ucsd.edu, apking@cs.ucsd.edu

Sutanu Sarkar, Eric Arobone, Hieu Pham
Department of Applied Mechanics and Engineering Sciences
University of California, San Diego
sarkar@ucsd.edu, earobone@gmail.com, h8pham@ucsd.edu

MS11
Use Reaction-Based Differential-Algebraic Equation Approach for Reactive Transport Modeling in Hydrologic Systems

We discuss how a reaction-based, differential-algebraic equation approach can provide robust numerical solutions for geochemical/biogeochemical systems that are composed of fast, slow, reversible, and irreversible reactions. We also discuss several numerical strategies for solving reactive transport equations using high performance computing.

Hwai-ping Cheng
US Army Engineer Research & Development Center
hwai-ping.cheng@usace.army.mil

Stacy Howington
US Army Engineer Research and Development Center

stacy.e.howington@usace.army.mil

MS11

Parallelization of a Vector-Optimized 3-D Flow Solver for Multi-Core Node Clusters

In order to increase feasible problem size, we have parallelized a vector-optimized 3-D flow solver for multi-core node clusters. MPI programming is used to manage the distribution of the computational grid across multiple nodes in the form of rectilinear slabs. For a problem size 512x256x256, running on a Cray XT4 and using 2 cores per node, the speed ratios for 32, 64, and 128 nodes are 1.00, 0.47 and 0.25. Key computational elements are LAPACK, FFTW, and a custom Poisson solver.

Bob Robins
Northwest Research Associates, Inc
bob@nwra.com

Gabriele Jost
Texas Advanced Computing Center
The University of Texas at Austin
gjost@tacc.utexas.edu

MS11

Lessons Learned in the Application of Distributed Memory Parallel Computing Systems For Computational Fluid Dynamics Analysis

A domain decomposition algorithm that has been used to develop a Navier-Stokes equations solver will be recapitulated. The interchange of messages between domains can be done by any message passing library. PVM and MPI message passing libraries have been employed successfully by this solver. Past experiences of running the solver on Cray T3D and T3E systems using PVM with up to 900 processors showed no difficulty in message passing. However, in an application of the solver on a cluster system (Beowulf) using MPI with 400 processors, several message passing difficulties were encountered. Two of the significant difficulties and the method of resolution will be presented in this paper. Events indicate that these difficulties occur at the interface between the MPI library and the operating/hardware system. Lessons learned and potential remedies will be discussed.

Johnson C. Wang
The Aerospace Corporation
Fluid Mechanics Department
johnson.c.wang@notes.aero.org

MS12

Should the Frequency of Screening Mammograms Depend on a Womans Age?

Breast tumors tend to grow faster in younger women, leaving a shorter window of opportunity for detecting breast cancer by mammography before it becomes symptomatic. In the absence of prospective trials, we used a mathematical model of breast cancer to address the question of whether screening frequency should depend on a womans age by running a Monte Carlo simulation comparing annual and biannual screening schedules for ages 40-54 and 55-70.

Linda Green
Archimedes
San Francisco, CA
linda.green@archimedesmodel.com

Tuan Dinh
Archimedes, Inc.
tuan.dinh@archimedesmodel.com

Robert Smith, James Kepner
American Cancer Society
robert.smith@cancer.org, james.kepner@cancer.org

MS12

Estimating the Likelihood of Cure from Lung Cancer

Lung cancer is the leading cause of death from cancer in the United States, yet screening for lung cancer is not recommended even for current and former smokers. Screening with a chest X-ray has not shown to be effective in reducing lung cancer mortality, and screening with a Computed Tomography (CT) examination is still under investigation. Even after the CT screening trail results are available, controversies regarding the interpretation of the results may persist for decades, as has been evidenced by the X-ray screening trials. At issue is our lack of knowledge on the natural history of lung cancer. It is not clear how quickly lung cancer progresses and how early it needs to be detected for cure. We propose a mathematical model of the natural history of lung cancer to estimate the relationship between the size of the primary tumor and the likelihood of cure. The model is applied separately to lung adenocarcinoma, squamous cell carcinoma, large cell carcinoma, and small cell carcinoma, and separately for males and females. Model parameters were estimated using data from the Surveillance, Epidemiology and End Results (SEER) cancer registry.

Sylvia Plevritis
Stanford University
Stanford, CA
sylvia.plevritis@stanford.edu

MS12

Computational Modeling in Design of Drug Eluting Stents

Coronary artery disease (CAD) is a leading cause of death in the US accounting for about half a million deaths every year (1 out of every 5.3 deaths). The use of stents in treating CAD has dramatically increased since their approval by the United States Food and Drug Administration in 1994. In order to overcome the problem of restenosis associated with the use of bare metal stents, drug-eluting stents (DES) were developed and subsequently introduced in the US in 2003. With the advent of DES, it has become critical to take into account a combinational perspective in designing stents. In addition to being mechanical scaffolds that hold open the arterial lumen, stents are also drug delivery devices that combat restenosis. Computational modeling has been extensively used in understanding cardiovascular mechanics and in designing therapies, such as stents, for treating cardiovascular disease. This presentation focuses on the use of computational modeling techniques for the design of DES. These techniques have been used in the research phase to investigate stent design concepts as well as to support regulatory filing to gain approval to commercialize these devices. Computational modeling has been used to evaluate the structural integrity of the stent platform, characterize the influence of the stent on arterial hemodynamics, study the drug release from stent coatings and understand the subsequent drug distribution in the arterial tissue. Knowledge gained using such modeling approaches serves as an input into the design of improved stent designs and next generation stent concepts.

Santosh Prabhu
Abbott Vascular
Santa Clara, CA
santosh.prabhu@av.abbott.com

MS12
New Phylogenomic Methods for Protein Function Prediction

Phylogenomic methods integrating genome information and phylogenetic reconstruction – are used for both the inference of species phylogenies and for the prediction of gene function. In this talk, I will discuss the explicit use of evolution as a fundamental principle in bioinformatics, using machine learning methods in combination with evolutionary models to improve the power and specificity of a number of bioinformatics tasks, including new methods from my group for orthology prediction, multiple sequence alignment, phylogenetic tree construction, and prediction of protein active site and specificity residues.

Kimmen Sjolander
UC Berkeley
Berkeley, CA
kimmen@berkeley.edu

MS13
Topology for Computer Generated Visual Effects

Visual effects in entertainment are produced from costly iterations of physically-based simulations for the purpose of achieving an artistically directed result. The technique of simulation alone is an insufficient tool for the effective execution of visual effects. Abstract mathematical notions are more helpful when directing stylized effects. Topology is a subfield of mathematics that permits the development of software that efficiently assists an artistically motivated user achieved a desired stylized effect.

Justin P. Bisceglio
Blue Sky Studios
University of Connecticut, Department of Computer Science
justin.bisceglio@gmail.com

MS13
Analysis on Triangulations

We apply tools of analysis directly to the vertices of a triangulation (of, for example, an image or a terrain) by systematically associating with each vertex a polynomial surface of degree equal to that of the vertex. Based, often just conceptually, upon this surface we carry out processes such as calculate curvature, classify critical points, or apply Gaussian smoothing kernels at a vertex using just the triangulation values at it and surrounding vertices.

Norman Noble
Kerner Graphics
San Rafael, CT
norm@metavideo.com

MS13
Modeling Knots for Aesthetics and Simulations

Knotted and linked structures play important roles in many fields, from modeling DNA molecules or wire-harnesses, to the creation of artistic sculptures and computer-generated movie scenes depicting entangled tentacles of some monster creatures. A theory of tubular neighborhoods guarantees that approximations and movements within such entangled regions will preserve crucial topological characteristics. Complementary computer engineering approaches are being developed to provide similar topological analysis, but which may permit more aggressive moves between subsequent simulation frames.

Carlo H. Sequin
EECS Computer Science Div.
U.C. Berkeley, CA, 94720-1776
sequin@cs.berkeley.edu

MS13
Level Sets for Imaging and Graphics

A variety of PDE-based image analysis, extraction and classification schemes have been developed in recent years, spanning topics such as medical imaging, data reduction, and configuration analysis. The author will describe recent work with applications to medical imaging, computer graphics, classification and pruning.

James Sethian
University of California, Berkeley
Department of Mathematics
sethian@math.berkeley.edu

MS14
Participant-driven Genetics Research at 23andMe

Despite the recent, rapid growth in genome-wide data, much of human variation remains entirely unexplained. A significant challenge in the pursuit of the genetic basis for variation in common human traits is the efficient, coordinated collection of genotype and phenotype data. We will present a web-based interface for this collection, explain how to minimize the biases inherent in this design, and present results of the analysis for several common traits.

Nick Eriksson
23andme
nick.eriksson@gmail.com

MS14
Transcription and Expression Dynamics in the Early Drosophila Embryo

We will explain the role of cis regulatory modules (CRMs) in the development of the early Drosophila embryo, and discuss competing mathematical models of gene expression driven by transcriptional control using such modules.

Lior Pachter
University of California, Berkeley
Dept. of Mathematics
lpachter@math.berkeley.edu

Anne Shiu
Department of Mathematics
UC Berkeley
annejls@berkeley.edu

Lester Mackey
Department of Computer Science
UC Berkeley
lmackey@eecs.berkeley.edu

MS14

Parsimonious Assembly of Shotgun Sequencing Reads via Dilworth's Theorem

Shotgun sequencing experiments randomly sample short substrings, called reads, of a much longer target DNA molecule. The target sequence must be computationally reconstructed or 'assembled' from these reads. In this talk, I will discuss the Cufflinks algorithm, which assembles a large population of messenger RNA sequences and also estimates the relative abundance of each sequence in the population. The algorithm imposes a partial ordering on the reads and assembles them into a parsimonious set of sequences via a constructive proof of Dilworth's Theorem. I will also briefly present data from our use of Cufflinks in an RNA sequencing experiment investigating embryonic muscle development in mouse. This is joint work with Geo Pertea, Ali Mortazavi, Brian Williams, Steven Salzberg, Barbara Wold, and Lior Pachter.

Cole Trapnell
University of Maryland, College Park
Department of Computer Science
cole@cs.umd.edu

MS14

Mathematical Modeling of Cancer-Immunology Dynamics

The critical importance of the immune system in combating cancer has been verified both clinically and through mathematical models. In this talk, we will discuss the biological and mathematical sides of the question of how cancer grows, how the cancer interacts with the immune system, and treatment approaches that harness the power of the immune system, including radiation, chemotherapy and immunotherapy. We will present computational solutions to models of various biological scenarios.

L. G. de Pillis
Harvey Mudd College
depillis@hmc.edu

MS15

The Claremont Mathematics Clinic: 36 years of Industrial Projects

The Claremont Mathematics Clinic, initiated in 1973, has completed 235 year-long projects to date for a variety of industrial, commercial and governmental clients. Each project runs two semesters and is staffed by 3-6 students who get course credit for their participation, and a faculty member. In addition the project requires close contact with client liaisons. We shall discuss clinic organization, report writing and presentation skills gained, success rates for the clients and students, etc.

Ellis Cumberbatch
Claremont Graduate University
Claremont, CA
ellis.cumberbatch@cgu.edu

MS15

Calculation of Geodesics on Piecewise Smooth Surfaces

I shall describe the clinic project undertaken by the CGU Math Clinic in 08-09, provided by Boeing. The problem was to find the geodesic connecting two points on a surface, composed of piecewise smooth sub-surfaces. The algorithm devised consists of evolving an initial curve that connects the two points so as to drive its geodesic curvature to zero throughout. Students: R. Caplan, M. Davis, J. Dehner, N. Hooper, H. Mattie; Liaison: T. Grandine; supported by NSF grant 0538663.

Ali Nadim
Claremont Graduate University
Department of Mathematics
ali.nadim@cgu.edu

MS15

Two Views of a Clinic Project: Student and Client Liaison

I will describe my experiences with the clinic program from the perspective of both a student and liaison. As a student, I worked on the 2006 Laserfiche clinic on computer assisted document classification, and as a liaison I represented Citadel Investment Group for our project on pairs trading. I will discuss how my time as a student prepared me for my career, how working as a liaison benefited Citadel, and how the clinic program sets Claremont graduates apart from other students entering the workforce.

Russell Osborn
Clarium Labs
rjosbo2@yahoo.com

MS15

Modeling Fluid Transport in Subcutaneous Tissue

The goal of this Cardinal Health project, conducted at HMC in 2008-09 by a math/physics team, is to produce a mathematical model of fluid flow in subcutaneous tissue. Two models have been developed: a compartment model that segregates the fluid into homogeneous regions, and a continuous model that describes the properties of the fluid at each point in space and time.

Rachel Levy, Richard Haskell, Stephen Rosenthal, Brian Stock, Melissa Strait, Harry Dudley
Harvey Mudd College
levy@math.hmc.edu, haskell@hmc.edu, srosenthal@hmc.edu, brian_stock@hmc.edu, melissa_strait@hmc.edu, harry_dudley@hmc.edu

Robert Butterfield
Cardinal Health
bob.butterfield@cardinalhealth.com

MS16

Quantifying Uncertainty In An Attempt To Answer Biomedical Questions: From The Computer Lab To The Clinic

Hypo-fractionated stereotactic body radiation therapy (SBRT) employs precisely-conforming high-level radiation dose delivery to improve tumor control probabilities and sparing of healthy tissue. However, the delivery precision and conformity of SBRT renders dose sparticularly susceptible to organ motion, and respiratory-induced motion in the abdomen may result in significant displacement of lesion targets during the breathing cycle. Given the maturity of the technology, sensitivity of dose deposition to respiratory-induced organ motion represents a significant factor in observed discrepancies between predictive treatment plan indicators and clinical patient outcome statistics and one of the major outstanding unsolved problems in SBRT. Techniques intended to compensate for respiratory-induced organ motion have been investigated, but very few have yet reached clinical practice. In this talk we discuss the challenges resuling from variability in dose deposition due to organ motion. To overcome these uncertainties and improve SBRT accuracy, it is essential to incorporate an accurate quantification of the effects of the random nature of the respiratory process on dose deposition into SBRT treatment planning systems. We introduce a means of characterizing the underlying day-to-day variability of patient breathing and calculate the resulting stochasticity in dose deposition using the polynomial chaos methodology.

Mike Kirby
School of Computing
University of Utah
kirby@sci.utah.edu

MS16

Statistical Inference and Experimental Design for Energy Conversion Processes

Detailed chemical kinetic and thermophysical models are essential to the design of complex energy conversion devices, from combustion engines to fuel cells. Yet significant uncertainties persist in the structure and parameters of these models. The rapid development of new fuels and energy conversion processes urges systematic approaches to model development that synthesize multiple sources of information and exploit indirect calibration data. In this context, we present efficient numerical methods for Bayesian inference using polynomial chaos expansions. We also present a Bayesian approach to optimal experimental design under uncertainty—choosing experimental conditions to maximize information gain in parameters or observables of interest.

Youssef M. Marzouk
Massachusetts Institute of Technology
ymarz@mit.edu

MS16

Uncertainty Quantification for Reactive Transport in Porous Media

Predictions of reactive transport in porous media are routinely compromised by both model (structural) and parametric uncertainties. We present a set of computational tools for quantifying these two types of uncertainty. The model uncertainty is resolved at the molecular scale where epistemic uncertainty incorporates aleatory uncertainty. The parametric uncertainty is resolved at both molecular and continuum (Darcy) scales. We use the proposed approach to quantify uncertainty in modeling the sorption of neptunium through a competitive ion exchange. We demonstrate how parametric and model uncertainties affect one's ability to estimate the distribution (partition) coefficient. The uncertainty quantification tools yield complete probabilistic descriptions of key parameters affecting the fate and migration of neptunium, rather than the lower statistical moments. This is important, since these distributions are highly skewed. We use such probabilistic parametrizations to derive a probability density function (pdf) formulation for advective transport of a solute that undergoes a heterogeneous chemical reaction involving an aqueous solution reacting with a solid phase. This system is described by a stochastic differential equation with multiplicative noise. We consider both linear and nonlinear kinetic rate laws, and derive an effective kinetic rate constant for the mean field approximation describing the change in mean concentration with time.

Daniel M. Tartakovksy
University of Carlifornia, San Diego
dmt@ucsd.edu

MS16

Efficient Numerical Algorithms for Uncertainty Quantification of Complex System

Recently there has been a surge of interest in developing efficient methods for simulation of complex systems subject to uncertain input. The source of uncertainty includes system parameters, initial and boundary conditions, geometry, etc. To ensure confidence in the simulation results one must consider the impact of the uncertainty from the beginning of the simulation. In this talk we review the current state-of-the-art of numerical development and focus on the methods suitable for large and complex systems.

Dongbin Xiu
Purdue University
dxiu@math.purdue.edu