IP1
Sparse Tensor Algorithms in Uncertainty Quantification

We survey recent mathematical and computational results on sparse tensor discretizations of Partial Differential Equations (PDEs) with random inputs. The sparse Tensor discretizations allow, as a rule, to overcome the curse of dimensionality in approximating infinite dimensional problems. Results and Methods surveyed include a) regularity and N-term gpc approximation results and algorithms for elliptic and parabolic PDEs with random coefficients [joint work with A. Cohen, R. DeVore and V.H.Hoang] and b) existence and regularity results for solutions of classes of certain hyperbolic PDEs from conservation and balance laws. Multi-Level Monte-Carlo (MLMC) [joint with A. Barth] and Multi-Level Quasi-Monte-Carlo (MLQMC) [joint with I. Graham, R. Scheichl, F.Y.Kuo and I.M. Sloan] methods can be viewed as particular classes of sparse tensor discretizations. Numerical MLMC and MLQMC results for elliptic PDEs with random coefficients and for nonlinear systems of hyperbolic conservation laws are presented [joint work with S. Mishra and J. Sukys (ETH)]. We compare the performance of these methods with that of adaptive generalized polynomial chaos discretizations.

Christoph Schwab
ETH Zuerich
SAM
christoph.schwab@sam.math.ethz.ch

IP2
Integrating Data from Multiple Simulation Models - Prediction and Tuning

Simulation of complex systems has become commonplace in most areas of science. In some settings, several simulators are available to explore the system, each with varying levels of fidelity. In this talk, Bayesian methodology for integrating outputs from multi-fidelity computer models, and field observations, to build a predictive model of a physical system is presented. The problem is complicated because inputs to the computer models are not all the same and the simulators have inputs (tuning parameters) that must be estimated from data. The methodology is demonstrated on an application from the University of Michigans Center for Radiative Shock Hydrodynamics.

Derek Bingham
Dept. of Statistics and Actuarial Science
Simon Fraser University
dbingham@cs.sfu.ca

IP3
Polynomial Chaos Approaches to Multiscale and Data Intensive Computations

Prediction of multiscale systems is increasingly being based on complex physical models that depend on large uncertain data sets. In this talk, we will outline recent developments in polynomial chaos (PC) methods for uncertainty quantification in such systems. Implementations will be illustrated in light of applications to chemical kinetics, and geophysical flows. Conclusions are in particular drawn concerning the potential of parallel databases in providing a platform for discovery, assessing prediction fidelity, and decision support.

Omar M. Knio

Duke University
omar.knio@duke.edu

IP4
Large Deviation Methods for Quantifying Uncertainty

Large deviation methods have been particularly successful in assessing small probabilities of rare events, which are difficult to compute. They are also at the center of many importance sampling methods that aim to estimate probabilities of rare events by Monte Carlo methods. Since probabilities of rare events are an important part of the emerging field of uncertainty quantification in complex scientific problems, the question arises as to how effective they are. This is because the results of large deviation theory depend sensitively on details of the probabilistic model used, and such details may not be available or may themselves be subject to uncertainty. I will address these issues with some examples using mean-field models and conservation laws and attempt to draw some broader conclusions.

George C. Papanicolaou
Stanford University
Department of Mathematics
papanico@math.stanford.edu

IP5
Model Reduction for Uncertainty Quantification of Large-scale Systems

Uncertainty quantification is becoming recognized as an essential aspect of development and use of numerical simulation tools, yet it remains computationally intractable for large-scale complex systems characterized by high-dimensional uncertainty spaces. In such settings, it is essential to generate surrogate models – low-dimensional, efficient models that retain predictive fidelity of high-resolution simulations. This talk will discuss formulations of projection-based model reduction approaches for applications in uncertainty quantification. For systems governed by partial differential equations, we demonstrate the use of reduced models for uncertainty propagation, solution of statistical inverse problems, and optimization under uncertainty.

Karen E. Willcox
Massachusetts Institute of Technology
kwillcox@MIT.EDU

IP6
Statistical Approaches to Combining Models and Observations

Numerical models and observational data are critical in modern science and engineering. Since both of these information sources involve uncertainty, the use of statistical, probabilistic methods play a fundamental role. I discuss a general Bayesian framework for combining uncertain information and indicate how various approaches (ensemble forecasting, UQ, etc.) fit in this framework. A paleoclimate analysis illustrates the use of simple physics and statistical modeling to produce inferences. A second example involves glacial dynamics and illustrates how updating models and data can lead to estimates of model error. A third example involves the extraction of information from multi-model ensembles in climate projection studies.

Mark Berliner

The Ohio State University
mb@stat.osu.edu

CP1
Capturing Signatures of *microcracks* from *macrolevel* Responses

The current work considers the problem of characterizing microcracks that are typically at 10–100 μm level (depending on the material). These microcracks are invisible to naked eyes, and can cause catastrophic failure once they grow to a certain critical length. A stochastic upscaling scheme based on previous work by Das is extended in the present work to include the effects of microcracks. The uncertainty (due to microstructural heterogeneities, and random size, orientation, and distribution of microcracks) is accounted for in the macroscopic (continuum) constitutive elasticity matrices by modeling them as bounded positive-definite random matrices. Distinct difference in probabilistic characteristics of macrolevel response variables is observed depending on the presence or absence of microcracks. This finding opens up a new way of capturing signatures of microcracks from macrolevel experimental response measurements.

Sonjoy Das, Sonjoy Das, Sourish Chakravarty
University at Buffalo
sonjoy@buffalo.edu, sonjoy@buffalo.edu, sc267@buffalo.edu

CP1
Identification of Uncertain Time-Dependent Material Behavior with Artificial Neural Networks

Reliability assessment of structures requires knowledge of the structural behavior. In case of new materials, tests are required to investigate structural behavior. Obtained measurements are usually limited and imprecise, which leads to difficulties in selecting or developing material models (stress-strain-time dependencies) and determine their parameters. In this work, we will present an alternative approach that is based on artificial neural networks. Recurrent neural networks are used to construct relationships between material-loads, and material-responses under uncertainty.

Steffen Freitag, Rafi L. Muhanna
Georgia Institute of Technology
steffen.freitag@gtsav.gatech.edu,
rafi.muhanna@gtsav.gatech.edu

CP1
Uncertainty Quantification of Discrete Element Micro-Parameters Conditioned on Sample Preparation of Homogeneous Particle Materials

This lecture analyzes the effect of varying micro-parameters of a Discrete Element Model (DEM) developed to analyze the effect of homogeneous particle materials. An experimental database is populated using steel spheres of constant diameter to build cylindrical specimens under controlled experimental conditions. Specimens vary from the loosest to the densest conditions. A 3D-DEM model is built to reproduce the same experimental sample preparation conditions, which is used to explore all varying micro-parameters combinations that lead to the reference experimental samples. X-Ray Computer Tomography is used to validate the numerical simulations.

Patrick R. Noble, Tam Doung
Texas A&M University
pnoble10@neo.tamu.edu, meokeen@tamu.edu

Zenon Medina-Cetina
Zachry Department of Civil Engineering
Texas A&M University
zenon@tamu.edu

CP1
Random Fields for Stochastic Mechanics of Materials

An approach based on a Hill-Mandel condition allows determination of scaling laws and mesoscale random fields with continuous realizations from the microstructural properties described by random fields with discontinuous realizations, typically given by image analyses of just about any microstructure. We discuss one- and two-point statistics of such fields, the (an)isotropy of realizations versus (an)isotropy of correlation functions, as well as their unavoidable scale-dependence, non-uniqueness, and correspondence with specific variational principles of solid mechanics.

Martin Ostoja-Starzewski
Department of Mechanical Science and Engineering
University of Illinois at Urbana-Champaign
martinos@uiuc.edu

Luis Costa
Institute for Multiscale Reactive Modeling
US Army ARL-ARDEC
luis.costa@us.army.mil

Emilio Porcu
Institute for Mathematical Stochastics
Georg-August-Universitaet, Goettingen, Germany
eporcu@uni-goettingen.de

CP1
Uncertainty Quantification in Image Processing

Based on the polynomial chaos and stochastic finite elements we construct stochastic extensions of image processing operators like Perona-Malik smoothing and Mumford-Shah resp. Ambrosio-Tortorelli segmentation and of the level set method. The stochastic extensions allow propagating information about the image noise from the acquisition step to the result, thus equipping the image processing results with reliability estimates. This modeling is important in medical applications where treatment decisions are based on quantitative information extracted from the images.

Torben Pätz
Jacobs University Bremen and Fraunhofer MEVIS
t.paetz@jacobs-university.de

Michael Kirby
University of Utah
School of Computing
kirby@cs.utah.edu

Tobias Preusser
Fraunhofer MEVIS, Bremen

tobias.preusser@mevis.fraunhofer.de

CP1
Statistics of Mesoscale Conductivities and Resistivities in Polycrystalline Graphite

We consider mesoscale heat conduction in random polycrystalline graphite under uniform essential (Dirichlet) and uniform natural (Neumann) boundary conditions. Using numerical experiments, we obtain rigorous bounds on all the six independent components of the mesoscale conductivity (and resistivity) tensor and thereby the three invariants. The bounds on conductivity obtained using the proposed approach are the tightest when compared to the Voigt, Reuss, upper and the lower Hashin-Shtrikman bounds and incorporate the effects of scaling unlike the other bounds. The scale-dependent probability densities of the invariants of the mesoscale conductivities (resistivities) are also determined.

Shivakumar I. Ranganathan
Department of Mechanical Engineering
American University of Sharjah
sranganathan@aus.edu

Martin Ostoja-Starzewski
Department of Mechanical Science and Engineering
University of Illinois at Urbana-Champaign
martinos@uiuc.edu

CP2
Model Discrepancy and Uncertainty Quantification

When quantifying uncertainty in computer models it is important to account for all sources of uncertainty. One important source of uncertainty is model discrepancy; the difference between reality and the computer model output. However, the challenge with incorporating model discrepancy in a statistical analysis of computer models is the confounding with calibration parameters. In this talk we explore, through examples, ways to include model discrepancy in a Bayesian setting.

Jenny Brynjarsdottir
Statistical and Applied Mathematical Sciences Institute
jenny.brynjarsdottir@gmail.com

Anthony O'Hagan
Univ. Sheffield, UK
a.ohagan@sheffield.ac.uk

CP2
Model Inadequacy Quantification for Simulations of Structures Using Bayesian Inference

We quantify the level of model inadequacy (aka model structure uncertainty) in simulations of the eigenfrequencies of a simple metal structure. Starting with a statistical model of the system, including parametric uncertainty, discretization error, as well as a generic representation of model inadequacy, we calibrate against an extensive experimental data-set, which includes attempts to identify and estimate sources of measurement noise and bias. A reliable estimate of model inadequacy for this simple situation is obtained.

Richard Dwight
Delft University of Technology

Netherlands
richard.dwight@gmail.com

Hester Bijl
Faculty Aerospace Engineering
Delft University of Technology, NL
h.bijl@tudelft.nl

CP2
Quantitative Model Validation Techniques: New Insights

This research develops new insights into quantitative model validation techniques. Traditional Bayesian hypothesis testing is extended based on interval hypotheses on distribution parameters and equality hypotheses on probability distributions. Two types of validation experiments (well characterized and partially characterized) are considered. It is shown that under some specific conditions, the Bayes factor metric in Bayesian equality hypothesis testing and the reliability-based metric can both be mathematically related to the p-value metric in classical hypothesis testing.

You Ling
Department of Civil and Environmental Engineering
Vanderbilt University
you.ling@vanderbilt.edu

Sankaran Mahadevan
Vanderbilt University
sankaran.mahadevan@vanderbilt.edu

CP2
Dynamic Model Validation of a 160 Mw Steam Turbine Lp Last Stage (L-0) Blade

Laboratory vibration testing of turbine blades has always provided a major contribution to the understanding, detection and the possibility to predict the probable failures encountered under real operation conditions. The importance of testing for large steam turbines, with long slender blades with increased risk of fatal vibrations, is higher due to cost and safety. In this regard, the main focus of this work is to identify the Siemens Co. benchmark blade modal model based on experimental test data, using SDOF and MDOF methods. The accuracy of the Circle and line fit methods were compared with a state-space subspace method called N4SID. Furthermore, in order to validate the smaller size model with capability to capture main features of the full model, SVD-based model approximation methods are used to achieve a minimal state space representation of the original model. Finally the accuracy and efficiency of a Hankel-norm based reduction and a balanced truncation method are compared and the results are presented.

Sadegh Rahrovani
Chalmers University of Technology
sadeghr@chalmers.se

Thomas Abrahamsson
Professor
thab@chalmers.se

Sadegh Sarvi
Senior Engineer
sarvi.sadegh@mapnaturbine.com

CP2
Quantifying Uncertainty and Accounting Model Discrepancy in Slider Air Bearing Simulations for Calibration and Prediction

Coupled multiphysics simulation of a slider air-bearing is routinely performed during a hard disk design process to achieve various critical performance requirements. Characterizing uncertainty through these simulations is critical to predict variation in outputs of interest and to drive sigma reduction of main contributing inputs. A non-intrusive sparse stochastic collocation scheme is used to propagate uncertainty here and its efficiency compared to the Latin hyper-cube Monte Carlo sampling approach. Experimental results are used to update unknown functions in the model inputs using a Bayesian formulation and Markov Chain Monte Carlo approach. In another specific application, the discrepancy between the simulation and the experimental results is accounted for by augmenting the model with discrepancy term and specifying a Gaussian Process model for the same. Two examples of applications in active fly height loss during environmental conditions and operational shock survival is presented here.

Ajaykumar Rajasekharan, Paul J Sonda
Mechanical Research & Development
Seagate Technology
ajaykumar.rajasekharan@seagate.com,
paul.j.sonda@seagate.com

CP2
Integration of Verification, Validation, and Calibration Activities for Overall Uncertainty Quantification

This talk presents a Bayesian methodology to integrate information from verification, validation, and calibration activities for overall prediction uncertainty quantification. Multi-level systems are considered, with two types of information flow - (1) lower-level output becomes higher-level input, and (2) parameters calibrated with lower-complexity models and experiments are applied to full system simulation. The various sources of uncertainty, multiple levels of models and experiments are connected through a Bayes network, to quantify the uncertainty in system-level prediction.

Shankar Sankararaman, Sankaran Mahadevan
Vanderbilt University
shankar.sankararaman@vanderbilt.edu,
sankaran.mahadevan@vanderbilt.edu

CP3
Dimension Reduction and Measure Transformation in Stochastic Multiphysics Modeling

We present a computational framework based on stochastic expansion methods for the efficient propagation of uncertainties through multiphysics models. The framework leverages an adaptation of the Karhunen-Loeve decomposition to extract a low-dimensional representation of information passed from component to component in a stochastic coupled model. After a measure transformation, the reduced-dimensional interface thus created enables a more efficient solution in a reduced-dimensional space. We demonstrate the proposed approach on an illustration problem from nuclear engineering.

Maarten Arnst
Universite' de Liege
maarten.arnst@ulg.ac.be

Roger Ghanem
University of Southern California
Aerospace and Mechanical Engineering and Civil
Engineering
ghanem@usc.edu

Eric Phipps
Sandia National Laboratories
Optimization and Uncertainty Quantification Department
etphipp@sandia.gov

John Red-Horse
Validation and Uncertainty Quantification Processes
Sandia National Laboratories
jrredho@sandia.gov

CP3
Contour Estimation Via Two Fidelity Computer Simulators under Limited Resources

In this work, we study the contour estimation problem for complex systems with two fidelity simulators. Using Gaussian process for surrogate construction, the sequential procedure is designed to choose the best suited simulator and input location for each simulation trial so that the overall estimation of the desired contour can be as good as possible under limited resources. Finally, the methodology is illustrated on a queueing system and its efficiency evaluated via a simulation study.

Ray-Bing Chen
Department of Statistics
National Cheng Kung University
rbchen@stat.ncku.edu.tw

Ying-Chao Hung
Department of Statistics
National Chengchi University
hungy@nccu.edu.tw

Weichung Wang
National Taiwan University
Department of Mathematics
wwang@math.ntu.edu.tw

Sung-Wei Yen
Department of Mathematics
National Taiwan University
r96221038@gmail.com

CP3
An Uncertainty Quantification Approach to Assess Geometry-Optimization Research Spaces through Karhunen-Loève Expansion

UQ is exploited to assess geometry-optimization research spaces and support the design of the optimization task. A set of prescribed geometries defines the research space through morphing. Karhunen-Loève Expansion gives the total geometric variance and the geometric variability of each principal direction. This is used to compare different spaces and reduce their dimension and the computational costs. Finally, UQ methods identify the statistical properties of the relevant objectives. Hydrodynamic application

in ship design is presented.

Matteo Diez
CNR-INSEAN, The Italian Ship Model Basin
m.diez@insean.it

Daniele Peri
INSEAN - The Italian Ship Model Basin
d.peri@insean.it

Frederick Stern
IIHR-Hydroscience and Engineering, The University of
Iowa
frederick-stern@uiowa.edu

Emilio Campana
INSEAN The Italian Ship Model Basin
e.campana@insean.it

CP3
Improvement in Multifidelity Modeling Using Gaussian Processes

Using different types of fidelity measurements can result in a large improvement of predictions by surrogate modeling in terms of computing time and precision. O'Hagan proposed an autoregressive Gaussian process to model the relationship between high and low accurate responses. However, we show that in practice the linearity is not always observed. Therefore in the present work the estimation of the relationship between the cheap and expensive responses by using smoothing splines is studied.

Celine Helbert
Laboratoire Jean Kuntzmann
University of Grenoble
celine.helbert@imag.fr

Federico Zertuche
University of Grenoble
FRANCE
zertuche@imag.fr

CP3
A Multiscale Framework for Bayesian Inference in Elliptic Problems

Motivated by applications in hydrology, we present a multiscale framework for efficient sampling of Bayesian posteriors. The method is broadly applicable, but we concentrate on length scales and a conditional independence structure defined by the multiscale finite element method. The problem has two key components: construction of a coarse-scale prior, and an iterative method for conditioning fine-scale realizations on coarse-scale constraints. Theoretical justification and numerical examples show that the framework can strongly decouple scales and lead to more efficient inference.

Matthew Parno, Youssef M. Marzouk
Massachusetts Institute of Technology
mparno@mit.edu, ymarz@mit.edu

CP4
Super Intrusive Polynomial Chaos for An Elliptic Pde for Heat Transfer

We study uncertainty quantification via an elliptic partial differential equation for certain heat transfer problems. We use a polynomial chaos formulation that is super intrusive – we use the structure of the equations to derive exact closed form expressions for the mean and standard deviation of a random field (verified via Monte Carlo simulation). We harness the problem specific stochastic dependence structure in a way that could be useful in a variety of other applications with a similar mathematical structure.

Andrew Barnes
General Electric
Global Research Center
barnesa@research.ge.com

Jose Cordova
General Electric Global Research Center
jose.cordova@ge.com

CP4
A Library for Large Scale Parallel Modeling and Simulation of Spatial Random Fields

Spatial random fields (RFs) model heterogeneous fields in computational simulations, including material properties, boundary/initial conditions, and geometric properties. We present a parallel API/library for modeling spatial RFs using either Karhunen-Loeve (KL) or Polynomial Chaos (PC) expansions. In addition to generating KL/PC realizations, the library includes a preprocessor to solve KL eigenproblems and a posteriori error estimators for the resulting approximate solutions. Finally we describe several applications, including structural mechanics and flow in porous media.

Brian Carnes
Sandia National Laboratories
bcarnes@sandia.gov

John Red-Horse
Validation and Uncertainty Quantification Processes
Sandia National Laboratories
jrredho@sandia.gov

CP4
Efficient Evaluation of Integral Quantities in Rdo by Sequential Quadrature Formulas.

Accuracy of the computation of the integral quantities involved in RDO represents a key element for the success of the optimization. If numerical quadrature is adopted, a convergence study of a benchmark UQ may be not sufficient, due to the changing characteristics of the objective function thru the optimization process. To preserve accuracy, different sequential quadrature formulas are here applied to a practical application for ship design, comparing their efficiency and the associated numerical effort.

Daniele Peri
INSEAN - The Italian Ship Model Basin
d.peri@insean.it

Matteo Diez
CNR-INSEAN, The Italian Ship Model Basin
m.diez@insean.it

CP4
Application of a Novel Adaptive Finite Difference Solution of The Fokker-Planck Equation for Uncer-

tainty Quantification

An accurate and computationally efficient intrusive approach for UQ is introduced. It utilizes the diffusionless Fokker-Planck equation for the time evolution of the PDF. This equation is solved numerically using a TVD finite difference scheme and a novel method for obtaining the grid distribution. The results for some time-dependent problems will be compared with exact solutions or other computational UQ methodologies to demonstrate the method's ability to accurately and efficiently obtain statistical quantities of interest.

Mani Razi, Peter Attar
School of Aerospace and Mechanical Engineering
University of Oklahoma
mani.razi-1@ou.edu, peter.attar@ou.edu

Prakash Vedula
University of Oklahoma
pvedula@ou.edu

CP4
Adjoint Error Estimation for Stochastic Collocation Methods

We use stochastic collocation on sparse grids for solving partial differential equations with random parameters. Our aim is to combine the method with an adjoint approach in order to estimate and control the error of some stochastic quantity, such as the mean or variance of a solution functional. Therefore, our major goal is to provide appropriate error estimates that require less computational effort then the collocation procedure itself.

Bettina Schieche
Graduate School of Computational Engineering, TU Darmstadt
Department of Mathematics, TU Darmstadt
schieche@gsc.tu-darmstadt.de

Jens Lang
Department of Mathematics
Technische Universität Darmstadt
lang@mathematik.tu-darmstadt.de

CP4
Robust Approximation of Stochastic Discontinuities

The robust approximation of discontinuities in stochastic problems is important, since they can lead to high sensitivities and oscillatory interpolations. To that end, we introduce finite volume robustness concepts from computational fluid dynamics into uncertainty quantification. The application of these new uncertainty propagation algorithms to engineering problems shows that they require a minimal number of samples to resolve discontinuities, for example, in transonic airfoil flow simulations with uncertain free stream conditions.

Jeroen Witteveen
Stanford University
Center for Turbulence Research
jasw@stanford.edu

Gianluca Iaccarino
Stanford University
jops@stanford.edu

CP5
Constrained Gaussian Process Modeling

In this paper, we introduce a new framework for incorporating constraints in Gaussian process modeling, including bound, monotony and convexity constraints. This new methodology mainly relies on conditional expectations of the truncated multinormal distribution. We propose several approximations based on correlation-free assumptions, numerical integration tools and sampling techniques. From a practical point of view, we illustrate how accuracy of Gaussian process predictions can be enhanced with such constraint knowledge.

Sebastien Da Veiga
IFP Energies nouvelles
sebastien.da-veiga@ifpenergiesnouvelles.fr

Amandine Marrel
CEA
amandine.marrel@cea.fr

CP5
A Learning Method for the Approximation of Discontinuous Functions in High Dimensions

Tractable uncertainty quantification in high dimensions requires approximating computationally intensive functions with fast and accurate surrogates. Functions exhibiting discontinuities or sharp variations with respect to their inputs cause significant difficulty for traditional approximation methods. We have developed an unstructured and sampling-based method to address such problems. First we locate discontinuities via a kernel SVM classifier and uncertainty sampling. Then we map each resulting smooth region to a regular domain on which to build sparse polynomial approximations utilizing existing theory.

Alex A. Gorodetsky
Massachussets Institute of Technology
goroda@mit.edu

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

CP5
Improvement of the Accuracy of the Prediction Variance Using Bayesian Kriging. Application to Three Industrial Case Studies.

Kriging is often used in computer experiments, in particular because it quantifies the variance of prediction which plays a major role in many applications (Efficient Global Optimization, Uncertainty Quantification, Sensitivity Analysis,...). In this talk we present three industrial case studies from different application fields (reservoir engineering, nuclear security, optics) where we show how bayesian kriging provides an accurate variance of prediction especially when prior information is available, for example when derived from less accurate but faster simulations.

Celine Helbert
Laboratoire Jean Kuntzmann
University of Grenoble
celine.helbert@imag.fr

CP5
Reduced Basis Surrogate Models and Sensitivity Analysis

Computation of Sobol indices requires a large number of runs of the considered model. These runs often take too much time, and one has to approximate the model by a surrogate model which is faster to run. We present a reduced basis method, a way to build efficient surrogate models, coming with a rigorous error bound certifying the model approximation, which can be used to provide an error estimation on the estimated Sobol indices.

Alexandre Janon, Maelle Nodet, Clémentine Prieur
LJK / Université Joseph Fourier Grenoble (France)
INRIA Rhône Alpes, France
alexandre.janon@imag.fr, maelle.nodet@inria.fr, clementine.prieur@imag.fr

CP5
Shape Invariant Model Approach to Functional Outputs Modelling

To tackle the problem of uncertainty propagation in dynamic simulators such as multiphase flow transport we propose a response surface method based on Gaussian Process. To reduce the dimension a shape invariant model approach is proposed. Multiple runs from the experimental design are modelled by a parametrical transformation applied to a template curve. The response surface model is then applied to the reduced set of transformation parameters from which the functional output is reconstructed.

Ekaterina Sergienko
University of Toulouse and IFP Energies Nouvelles
ekatarina.sergienko@ifpen.fr

Fabrice Gamboa
Laboratory of Statistics and Probability
University of Toulouse
fabrice.gamboa@math.univ-toulouse.fr

Daniel Busby
IFP Energies Nouvelles
daniel.busby@ifpen.fr

CP5
Svr Regression with Polynomial Kernel and Monotonicity Constraints

Very often, regression models have to respect some additionnal constraints like monotonicity constraints. We present here a new method based on Support Vector Regression and Polynomial Kernel. As a major feature this method produces an equation valid in the whole domain of interest, which can be used without any additionnal work by engineers. Avoiding any discretization of the domain, this method can be applied up to 10 regressions variables.

Francois Wahl
IFPEN
Francois.wahl@ifpen.fr

CP6
Quantification of Uncertainty of Low Fidelity Mod-

els and Application to Robust Design

One of the major difficulties concerning uncertainty propagation techniques is to identify and quantify the sources of uncertainty. Predictive uncertainty of models has been defined as the main source of uncertainty in aircraft preliminary design. Moreover, its quantification is made more complex by model interdependencies. The aim of this study is to propose a way to quantify model predictive uncertainty and propagate it through an overall design process to figure out the robustness of its result.

Jessie Birman
Airbus Operation S.A.S.
jessie.birman@airbus.com

CP6
Path Variability Due To Sensor Geometry

The concept of Path Variability Due To Sensor Geometry (PVDSG) is fundamental to geomatic engineering. The PVDSG is a measure of the variability "built into' a statistic based on the distances from a target to the elements of a sensor array, due to the particular geometry of that array, as the target traverses a given path. This paper documents PVDSG measures as functions of the covariance matrix of the proportional target/sensor separations.

Timothy Hall
PQI Consulting
info@pqic.com

CP6
Risk-Averse Control of Linear Stochastic Systems with Low Sensitivity: An Output-Feedback Paradigm

The research investigation treats the problem of controlling stochastic linear systems with quadratic criteria, including sensitivity variables is investigated, when noisy measurements are available. It is proved that the low sensitivity control strategy with risk aversion can be realized by the cascade of: i) the conditional-mean estimates of the current states using a Kalman filter and ii) optimally feedback, which is comprised of a custom set of mathematical statistics associated with the finite-horizon quadratic random cost. In other words, the certainty equivalence principle still holds for this class of optimal statistical control problem.

Khanh D. Pham
The Air Force Research Laboratory
Space Vehicles Directorate
khanh.pham@kirtland.af.mil

CP6
An Information-Based Sampling Scheme with Applications to Reduced-Order Modeling

This work presents a novel methodology to sample effectively relevant points in the parameter space when designing computer experiments, or collecting snapshots for reduced-order models from an expensive to evaluate computer model. Principles from *information geometry* are employed, where the parameter space is interpreted as a Riemannian manifold equipped with a sensitivity related metric. An adaptive Sequential Monte Carlo scheme enables an effective sampling of such points, while allowing a controlled computational cost related to the evaluations of

the computer model. Numerical examples, in the context of reduced order modeling, are provided.

Raphael Sternfels
School of Civil & Environmental Eng, Cornell University
hrs63@cornell.edu

Christopher J. Earls
Cornell University
cje23@cornell.edu

CP7
A Method for Solving Stochastic Equations by Reduced Order Models

A method is developed for calculating statistics of the solution U of a stochastic equation depending on an R^d-valued random variable Z. The method is based on two recent developments. The first approximates the mapping $Z \mapsto U(Z)$ by a finite family of hyperplanes tangent to $U(Z)$ at points selected by geometrical considerations. The second represents Z by a simple random vector $\tilde{Z}$ delivered by an optimization algorithm minimizing the discrepancy between properties of Z and $\tilde{Z}$. The methods uses samples of $\tilde{Z}$ to construct approximate representations for $U(Z)$, so that these representations account for the probability law of Z.

Mircea Grigoriu
School of Civil Engineering
Cornell University
mdg12@cornell.edu

CP7
Effect of Limited Measurement Data on State and Parameters Estimation in Dynamic Systems

This work characterizes the effect of data uncertainty on estimates of state and parameters of dynamic systems. The sample moments of state and parameters of dynamic system based on limited available measurements are treated as random variates that characterize the effects of uncertainty due to limited measurement data. The Hankel matrices associated with each sample moment estimator (that arises in the context of corresponding Hamburger moment problem) and the covariance matrix (that characterizes statistical dependencies among the sample moment estimators), thus, turn out to be random positive-definite matrices. An array of methodologies (Bayes' theorem, random matrix theory, maximum entropy principle, and polynomial chaos expansion) are employed to estimate the probability density functions of these positive-definite random matrices. Efficient sampling schemes are also presented to sample from these pdfs.

Sonjoy Das, Sonjoy Das, Reza Madankan
University at Buffalo
sonjoy@buffalo.edu, sonjoy@buffalo.edu,
rm93@buffalo.edu

Puneet Singla
Mechanical & Aerospace Engineering
University at Buffalo
p.singla@gmail.com

CP7
Managing Uncertainty in Complex Dynamic Mod-els

Various fields of science/engineering have developed application specific formulations of uncertainty quantification with computational approaches. Such efforts in control system analysis employ functional analysis and semidefinite programming, yielding tractable algorithms for quantifying the effect of individual component uncertainty and unknown external influences on behavior of large, heterogeneous interconnections of components. This talk will review the formalism, its use in practice, and explore the potential connections across other areas to better exploit each other's successes.

Ufuk Topcu
Caltech
utopcu@cds.caltech.edu

Peter Seiler
U of Minnesota
peter.j.seiler@gmail.com

Michael Frenklach
University of California at Berkeley
myf@me.berkeley.edu

Gary Balas
U of Minnesota
balas@aem.umn.edu

Andrew Packard
U of California at Berkeley
apackard@berkeley.edu

CP7
On-Line Parameter Estimation and Control of Systems with Uncertainties

We present a method for parameter estimation and control of dynamical systems with uncertainties in real time. The method combines the polynomial chaos (PC) theory for uncertainty propagation and the Bayesian framework for parameter estimation in a novel way. The recursive nature of the algorithm requires the estimation of the PC coefficients of the parameters from their posterior distribution. We present methods for estimating these coefficients. The problem is motivated by a biological application.

Faidra Stavropoulou
Helmholtz Zentrum Muenchen
faidra.stavropoulou@mytum.de

Johannes Mueller
TU Muenchen
johannes.mueller@mytum.de

CP7
Estimation and Verification of Curved Railway Track Geometry Using Monte Carlo Particle Filters

A railway track geometry differs from the pre-designed one. It has track irregularities due to the frequent traffic of the train. A railway track geometry of level and alignment is measured based on the principle of three-point chord measurement, called 10m chord versine. Reconstructing the true track geometry from the measured data is a kind of the inverse problem. In this study a method of estimating

and verifying the true track geometry in the curved section from measured data using Monte Carlo particle filters is described.

Akiyoshi Yoshimura
Tokyo University of Technology
Emeritus Professor
aki-yoshimura@kyi.biglobe.ne.jp

CP8
Investigations on Sensitivity Analysis of Complex Final Repository Models

The complex computation models for assessing the long-term safety of final repositories for radioactive waste typically show a number of particularities that can cause problems when a probabilistic sensitivity analysis is performed, such as skewed output distributions over many orders of magnitude, including the possibility of zero-output, or non-continuous behavior. Several numerical experiments are presented, demonstrating these problems and some ideas to deal with them. Different correlation-based and variance-based techniques of sensitivity analysis are applied and compared.

Dirk-Alexander Becker
Gesellschaft fuer Anlagen- und Reaktorsicherheit (GRS) mbH
dirk-alexander.becker@grs.de

CP8
Global Sensitivity Analysis for Disease and Population Models

Variance based sensitivity measures are used to examine the structure of biological models. To limit expensive model evaluations we use a Gaussian process emulator to estimate sensitivity indices. The use of a stochastic surrogate model allows us to quantify the uncertainty due to lack of data in sensitivity estimates. Our methods are applied to an ODE based model for the spread of an epidemic on a network and to an agent based model of disease in a metropolitan region.

Kyle S. Hickmann, James (Mac) Hyman, John E. Ortmann
Tulane University
khickma@tulane.edu,   mhyman@tulane.edu,
jortmann@tulane.edu

CP8
A Global Sensitivity Analysis Method for Reliability Based Upon Density Modification

For global sensitivity analysis of numerical models, variance decomposition is widely applied. However, when the quantity of interest is a failure probability this method requires numerous function evaluations and does not always provide relevant information . We propose a new importance sampling method based upon modification of the distribution of inputs controlled by Kullback-Leibler divergence. The function sample is evaluated only once, resulting in significant time saving.

Paul Lematre
EDF R&D
INRIA Bordeaux
paul.lemaitre@edf.fr

Ekaterina Sergienko
University of Toulouse and IFP Energies Nouvelles
ekatarina.sergienko@ifpen.fr

Fabrice Gamboa
Laboratory of Statistics and Probability
University of Toulouse
fabrice.gamboa@math.univ-toulouse.fr

Bertrand Iooss
EDF R&D
bertrand.iooss@edf.fr

CP8
Fast and Rbd Revisited

This is a new introduction to the existing ANOVA-based global sensitivity analysis methods: Fourier Amplitude Sensitivity Test (FAST) and Random Balance Design (RBD). First this work consists in clarifying the underlying mathematical theory, then in performing a rigorous error analysis and last in suggesting some improvements and generalizations of both these methods. Numerical examples are also provided to illustrate this work.

Jean-Yves Tissot
University of Grenoble - INRIA
jean-yves.tissot@imag.fr

Clémentine Prieur
LJK / Université Joseph Fourier Grenoble (France)
INRIA Rhône Alpes, France
clementine.prieur@imag.fr

CP8
Locality Aware Uncertainty Quantification and Sensitivity Algorithms

A need exists for UQ and sensitivity analysis algorithms that leverage information from one system realization to another. Although the size of the computational models used in many engineering and scientific simulations is extremely large, *i.e.* millions of equations, the uncertainty present is oftentimes very localized to small regions of the model. Here, recent efforts to develop computational methods that exploit this localization and the ensemble nature of the requisite iterative analyses will be discussed.

Steven F. Wojtkiewicz
Department of Civil Engineering
University of Minnesota
ykvich@umn.edu

Erik A. Johnson
Astani Dept of Civil & Env Engrg
University of Southern California
johnsone@usc.edu

CP9
Emulating Dynamic Models - Numerical Challenge

Dynamic models can be emulated by linearizing its equations and compensating for the non-linearities with Gaussian white noise. Coupling replica of the resulting linear stochastic system according to the distance between their inputs and conditioning the coupled system on off-line simulation outputs results in a mechanistic emulator. For piece-wise constant inputs, the covariance matrix of

the coupled system can be derived explicitly. Conditioning of the emulator boils down to an (off-line) inversion of this covariance matrix and the emulation to mere (on-line) multiplications of matrices of the dimension of the state space. This approach is compared with Kalman filtering and smoothing.

Carlo Albert
Eawag
carlo.albert@eawag.ch

CP9
Multi-Modal Oil Reservoir History Matching Using Clustered Ensemble Kalman Filter

A multi-modal history-matching algorithm using Regularized Ensemble Kalman Filter was developed. The EnKF algorithm is augmented with k-means clustering algorithm to form sub-ensembles that explore different parts of the search space. Clusters are updated at regular intervals to merge clusters approaching the same local minima. The resulting mean of each sub-ensemble is used for robust production optimization. The proposed algorithm provides an efficient method for parameter estimation, uncertainty quantification and robust optimization of oil production.

Ahmed H. ElSheikh
Department of Earth Science and Engineering
Imperial College London, South Kensington Campus
a.el-sheikh@imperial.ac.uk

CP9
A Spectral Approach to Linear Bayesian Updating

The linear Bayesian methods of the family of low-rank Kalman filters have become popular for the solution of inverse and data assimilation problems, with one example being the ensemble Kalman filter. In this work we present a related approach which is based on well-known spectral expansions of the stochastic space, like the polynomial chaos expansion. The connection of this 'Bayes linear' approach with the original Bayes formula is highlighted, an it is demonstrated that spectral expansions can be used directly in the update equation without any detour to sampling. Numerical examples show the advantages and challenges of this approach. Examples will be given involving the well-known Lorenz systems and the estimation of a diffusion coefficient.

Oliver Pajonk
Institute of Scientific Computing
Technische Universität Braunschweig
o.pajonk@tu-bs.de

Bojana V. Rosic
Institute of Scientific Computing
TU Braunschweig
bojana.rosic@tu-bs.de

Alexander Litvinenko
TU Braunschweig, Germany
litvinen@tu-bs.de

Hermann G. Matthies
Institute of Scientific Computing
Technische Universität Braunschweig
wire@tu-bs.de

CP9
Uncertainty Quantification in the Ensemble Kalman Filter

The Ensemble Kalman Filter (EnKF) is a data assimilation algorithm that over the last decade has been applied to numerous fields. However, it is well known that the standard implementation of the EnKF will lead to an underrepresentation of the prediction uncertainty. In this talk we will explain, using classical results from statistics, why the EnKF is not able to quantify the uncertainty correctly, and present statistical methods that can resolve this issue.

Jon Saetrom
Statoil ASA
jonsat@statoil.com

Henning Omre
Norwegian University of Science and Technology
omre@math.ntnu.no

CP9
Collocation Inference for Nonlinear Stochastic Dynamic Systems with Noisy Observations

Collocation-based methods are proposed for estimating parameters and performing inference for nonlinear stochastic continuous-time dynamic systems with noisy observations. EM algorithm is applied to handle the systematic stochastic input and the observational error simultaneously. The approaches use collocation method to avoid the computational intensity. Two computation algorithms: Laplace approximations and Monte Carlo integration are examined. The convergence rates are h^p, where h is the bandwidth of the approximation scheme for stochastic Ronge-Kutta type penalty.

Yuefeng Wu
Department of Applied Mathematics and Statistics
University of California Santa Cruz
yuefeng@soe.ucsc.edu

Giles Hooker
Biostatistics and Computational Biology Department
Cornell University
giles.hooker@cornell.edu

CP10
Langevin Based Inversion of Pressure Transient Testing Data

In the oilfield, pressure transient testing is an ideal tool for determining average reservoir parameters, but this technique does not fully quantify the uncertainty in the spatial distribution of these parameters. We wish to determine plausible parameter distributions, consistent with both the pressure transient testing data and prior geological knowledge. We used a Langevin-based MCMC technique, adapted to the large number of parameters and data, to identify geological features and characterize the uncertainty.

Richard Booth, Kirsty Morton
Schlumberger Brazil Research and Geoengineering Center
RBooth2@slb.com, kmorton@slb.com

Mustafa Onur
Istanbul Technical University
onur@itu.edu.tr

Fikri Kuchuk
Schlumberger Riboud Product Center
kuchuk1@slb.com

CP10
Some Inverse Problems for Groundwater

Perhaps the most appealing aspect of Bayesian inference in the context of groundwater engineering is that it makes proper use of data, and provides the engineer with a tool that may be used to inform the judicious design of pump tests so that quantities of interest are determined within acceptable bounds. Low dimensional inverse problems for groundwater may capture the essential physics and provide guidance on what is important in the solution of their higher dimensional cousins; we present some recent work on low and high dimensional inverse problems for groundwater.

Nicholas Dudley Ward
Otago Computational Modelling Group
nick@ocmo.co.nz

Tiangang Cui
University of Auckland
tcui001@aucklanduni.ac.nz

Jari P Kaipio
Department of Applied Physics, University of Eastern Finland
2Department of Mathematics, University of Auckland
jari@math.auckland.ac.nz

CP10
Bayesian Acoustic Wave-Field Inversion of a 1D Heterogeneous Media

We discuss a Bayesian parameter estimation scheme to reconstruct the distribution of the subsurface elastic characteristics of a 1D heterogeneous earth model, given the probed medium's response to interrogating acoustic waves measured at the surface. We consider a generic multilayer media where the number of layers along with their velocities and thicknesses are treated as random variables, where the solution's non-uniqueness is fully accounted for by the posterior probability density of the unknowns. A synthetic study is provided to indicate the applicability of the technique.

Saba S. Esmailzadeh
Zachry Department of Civil Engineering,
Texas A&M University, College Station, TX, USA 77840
saba61@neo.tamu.edu

Zenon Medina-Cetina
Zachry Department of Civil Engineering
Texas A&M University
zenon@tamu.edu

Jun Won Kang
Department of Civil Engineering
New Mexico State University, NM 88003, USA.
jwkang@nmsu.edu

Loukas F. Kallivokas
The University of Texas at Austin
loukas@mail.utexas.edu

CP10
Inverse Problem: Information Extraction from Electromagnetic Scattering Measurement

The estimation of local radioelectric properties of materials from the global electromagnetic scattering measurement is a challenging ill-posed inverse problem. It is intensively explored on High Performance Computing machines by a Maxwell solver and statistically reduced to a simpler probabilistic metamodel. Considering the properties as a dynamic stochastic process, it is shown how advanced Markov Chain Monte Carlo methods, called interacting Kalman filters, can perform Bayesian inference to estimate the properties and their associated uncertainties.

Pierre Minvielle-Larrousse, Marc Sancandi, FranÇois Giraud, Pierre Bonnemason
CEA, DAM, CESTA
pierre.minvielle@cea.fr, marc.sancandi@cea.fr, francois.giraud@cea.fr, pierre.bonnemason@cea.fr

CP10
Set-Based Parameter and State Estimation in Nonlinear Differential Equations Using Sparse Discrete Measurements

Bounded experimental uncertainty and sparse measurements limit our ability to generate estimates of component concentrations and kinetic parameters in biological models because of algorithm instability and computational intractability. We present a set-based approach for producing estimates that address these issues. We use first-principles and a-priori knowledge to generate stabilizing bounds that maintain algorithm stability while removing spurious solutions that occur due to limited measurements. This is implemented in a multithreaded architecture to address computational limitations.

Cranos M. Williams, Skylar Marvel
North Carolina State University
cmwilli5@ncsu.edu, swmarvel@ncsu.edu

CP10
Probabilistic Solution of Inverse Problems under Varying Evidence Conditions

Results of the impact of varying evidence conditions on the probabilistic calibration of model parameters are presented. A synthetic case study is populated where data is fully controlled, including the effect of location, number, variance and correlation, when used to calibrate a simple differential equation used to simulate diffusion problems. Since the calibration follow a Bayesian approach, it is thus possible to describe the uncertainty changes on the model parameters as the evidence conditions vary, as this is reflected on independent analyses of the posterior distribution.

Zenon Medina Cetina, Negin Yousefpour
Texas A&M University
zmedina@civil.tamu.edu, neginyousefpour@gmail.com

Hans Petter Langtangen, Are Magnus Bruaset, Stuart Clark
Simula Research Laboratory
hpl@simula.no, arem@simula.no, stuart@simula.no

CP11
Adaptive Error Modelling in Mcmc Sampling for Large Scale Inverse Problems

We present a new adaptive delayed-acceptance MCMC algorithm (ADAMH) that adapts to the error of a reduced order model to enable efficient sampling from the posterior distribution arising in large scale inverse problems. This use of adaptivity differs from existing algorithms that tune the proposals, though ADAMH also implements that. Conditions given by Roberts and Rosenthal (2007) are used to give constructions that are provably convergent. We applied ADAMH to several large scale groundwater studies.

Tiangang Cui
University of Auckland
tcui001@aucklanduni.ac.nz

Nicholas Dudley Ward
Otago Computational Modelling Group
nick@ocmo.co.nz

Colin Fox
University of Otago, New Zealand
fox@physics.otago.ac.nz

Mike O'Sullivan
The University of Auckland
m.osullivan@auckland.ac.nz

CP11
Scalable Methods for Large-Scale Statistical Inverse Problems, with Applications to Subsurface Flow

We address the challenge of large-scale nonlinear statistical inverse problems by developing an adaptive Hessian-based non-stationary Gaussian process response surface method to approximate the posterior pdf solution. We employ an adaptive sampling strategy for exploring the parameter space efficiently to find interpolation points and build a global analytical response surface far less expensive to evaluate than the original. The accuracy and efficiency of the response surface is demonstrated with examples, including a subsurface flow problem.

H. Pearl Flath
Institute for Computational Engineering and Sciences
The University of Texas at Austin
pflath@ices.utexas.edu

Tan Bui-Thanh
The University of Texas at Austin
tanbui@ices.utexas.edu

Omar Ghattas
University of Texas at Austin
omar@ices.utexas.edu

CP11
Chemical Reaction Mechanism Generation Using Bayesian Variable Selection

The generation of detailed chemical reaction mechanisms, for applications ranging from electrochemistry to combustion, must often rely on noisy and indirect system-level data. We present a novel approach to mechanism generation based on Bayesian variable selection and a PDE-based physical model. Adaptive Markov chain Monte Carlo methods are used to efficiently explore a posterior that encompasses models comprised of subsets of elementary reactions. In contrast to conventional techniques, our approach provides a statistically rigorous assessment of uncertainty in reaction mechanism structure and in reaction rate parameters.

Nikhil Galagali, Youssef M. Marzouk
Massachusetts Institute of Technology
nikhilg1@mit.edu, ymarz@mit.edu

CP11
Inferring Bottom Bathymetry from Free-Surface Flow Features

We are solving an inverse problem of determining bathymetry of a channel from the mean flow features at the free surface. Our approach is optimization-based operating on a database of simulations with parameterized bedforms. Sensitivity of the inversion process to noise (e.g., instrument error, turbulence) is investigated. In the present framework, we rely on the time-averaged surface flow features, although also consider a more complex problem of using multiple free-surface snapshots of the unsteady flow.

Sergey Koltakov, Gianluca Iaccarino
Stanford University
koltakov@stanford.edu, jops@stanford.edu

Oliver Fringer
Environmental Fluid Mechanics Laboratory
Stanford University
fringer@stanford.edu

CP11
Bayesian Updating of Uncertainty in the Description of Transport Processes in Heterogeneous Materials

The prediction of thermo-mechanical behaviour of heterogeneous materials such as heat and moisture transport is strongly influenced by the uncertainty in parameters. Such materials occur e.g. in historic buildings, and the durability assessment of these therefore needs a reliable and probabilistic simulation of transport processes, which is related to the suitable identification of material parameters. In order to include expert knowledge as well as experimental results, we employ a Bayesian updating procedure.

Jan Sykora
Faculty of Civil Engineering
Czech Technical University in Prague
jan.sykora.1@fsv.cvut.cz

Anna Kucerova
Faculty of Civil Engineering, Prague, Czech TU
anicka@cml.fsv.cvut.cz

Bojana V. Rosic
Institute of Scientific Computing
TU Braunschweig
bojana.rosic@tu-bs.de

Hermann G. Matthies
Institute of Scientific Computing
Technische Universität Braunschweig
wire@tu-bs.de

CP12

Bayesian Models for the Quantification of Model Errors in Pde-Based Systems

Bayesian formulations offer a unified statistical treatment for the solution of model-based inverse problems. Apart from the noise in the data, another source of uncertainty, which is largely unaccounted for, is model uncertainty.In general, there will be deviations between the physical reality where measurements are made, and the idealized mathematical/computational description (in our case a system of PDEs consisting of conservation laws and constitutive equations). We propose an intrusive Bayesian strategy and efficient inference tools that are capable of quantifying model errors in the governing equations.

Phaedon S. Koutsourelakis
Heriot Watt University
P.Koutsourelakis@hw.ac.uk

CP12

Predictive Simulation for CO2 Sequestration in Saline Aquifers

One of the most difficult tasks in CO2 sequestration projects is the reliable characterization of properties of the subsurface. A typical situation employs dynamic data integration such as sparse CO2 measurement data in time and sparse measurements of permeability and porosity in space to be matched with simulated responses associated with a set of permeability and porosity fields. Among the challenges found in practice are proper mathematical modeling of the flow, persisting heterogeneity in porosity and permeability, and the uncertainties inherent in them. In this talk, we propose a Bayesian framework Monte Carlo Markov Chain simulation (MCMC) to sample a set of characteristics of the subsurface from the posterior distribution that are conditioned to the measured CO2 data. This process requires obtaining the simulated responses over many iterations. We use the model proposed in Obi and Blunt [Water Resources Research, 2006] to perform numerical simulations of the injection of CO2 in saline aquifers, and illustrate the MCMC procedure and its use in predictive simulation for CO2 sequestration.

Victor E. Ginting, Marcos Mendes
Department of Mathematics
University of Wyoming
vginting@uwyo.edu, marcosalcoforado@gmail.com

Felipe Pereira
Center for Fundamentals of Subsurface Flow
University of Wyoming
lpereira@uwyo.edu

Arunasalam Rahunanthan
Center for Fundamentals of Subsurface Flow
University of Wyoming, Laramie, WY 82071
rahu@uwyo.edu

CP12

The Effect of Prediction Error Correlation on Bayesian Model Updating

In this contribution, a Bayesian inference framework is adopted to quantify uncertainties due to measurement and modeling errors in vibration-based model updating. In most cases, independent normal distributions are assumed for the observed prediction errors on natural frequencies and mode shape components. However, such an assumption is not expected to hold in case of mode shape components identified from dense sensor networks. A correlated prediction error is therefore introduced and its effect on the identification is investigated.

Ellen Simoen
K.U.Leuven
ellen.simoen@bwk.kuleuven.be

Costas Papadimitriou
University of Thessaly
Dept. of Mechanical Engineering
costasp@uth.gr

Guido De Roeck, Geert Lombaert
K.U.Leuven
Dept. of Civil Engineering
guido.deroeck@bwk.kuleuven.be,
geert.lombaert@bwk.kuleuven.be

CP12

Investigating Uncertainty in Aerothermal Model Predictions for Hypersonic Aircraft Structures

Validating computational models of fluid-thermal-structural interactions in hypersonic aircraft structures remains a challenge due to limited experimental data. This research investigates uncertain model parameters and model errors in aerodynamic pressure and heating predictions. The modeled conditions correspond to aerothermal test data from hypersonic wind tunnel experiments of a spherical dome protuberance on a flat plate. Bayesian calibration and sensitivity analysis are used with the test data to improve understanding of model and experimental uncertainty.

Benjamin P. Smarslok
Air Force Research Laboratory
benjamin.smarslok@wpafb.af.mil

Sankaran Mahadevan
Vanderbilt University
sankaran.mahadevan@vanderbilt.edu

CP13

Reservoir Uncertainty Quantification Using Clustering Methods

Quantifying uncertainty in reservoir predictions is important in the petroleum industry, since more accurate quantification of the uncertainty contributes to prudent multimillion dollar decision makings. Nowadays predictions are made from conditioned multi-model ensembles obtained in history-matching using optimisation with evolutionary algorithms. These ensembles are usually multi-modal and different models will result in different forecasts. We use k-mean, probabilistic distance, and agglomerate clustering methods to locate and track multiple distinct optima representing uncertainties of the reservoir.

Asaad Abdollahzadeh
Heriot-Watt University
asaad.abdollahzadeh@pet.hw.ac.uk

Mike Christie
Heriot-Watt University, UK
Mike.Christie@pet.hw.ac.uk

David W. Corne
Heriot-Watt University
d.w.corne@hw.ac.uk

CP13
Adaptive Smolyak Pseudospectral Expansions

Smolyak pseudospectral expansions provide an efficient and accurate approach for computing sparse polynomial chaos approximations of functions with weak coupling between the input dimensions. We rigorously develop the Smolyak algorithm and show that it is well behaved. This behavior stands in contrast to the traditional sparse quadrature approach for building polynomial expansions, which is either inaccurate or inefficient in almost all cases. Furthermore, we tailor the Smolyak algorithm to individual functions at run-time through an adaptive strategy.

Patrick R. Conrad
MIT
prconrad@mit.edu

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

CP13
Uncertainty and Differences in Global Climate Models

Climate models have greatly aided investigation of global climate change. The uncertainty, similarities, and differences between climate models can be examined using exceedance regions. We propose methodology for drawing conclusions about entire exceedance regions with known confidence. The methodology uses kriging and conditional simulation to create confidence regions having the necessary statistical properties. Discussion will include assessment of future climate change for several regions of North America and highlight differences between various climate models.

Joshua P. French
University of Colorado Denver
joshua.french@ucdenver.edu

Stephan Sain
Institute for Mathematics Applied to Geosciences
National Center for Atmospheric Research
ssain@ucar.edu

CP13
Comparison of Stochastic Methods for Bayesian Updating of Uncertainty in Parameters of Nonlinear Models

An extensive development of efficient methods for stochastic modelling enabled uncertainty propagation through complex models. In this contribution, we present a review and comparison of several approaches such as stochastic Galerkin method or stochastic collocation method in context of Bayesian uncertainty updating.

Anna Kucerova
Faculty of Civil Engineering, Prague, Czech TU
anicka@cml.fsv.cvut.cz

Jan Sykora
Faculty of Civil Engineering
Czech Technical University in Prague
jan.sykora.1@fsv.cvut.cz

Bojana V. Rosic
Institute of Scientific Computing
TU Braunschweig
bojana.rosic@tu-bs.de

Hermann G. Matthies
Institute of Scientific Computing
Technische Universität Braunschweig
wire@tu-bs.de

CP13
Stochastic Anova-Galerkin Projection Schemes

We present numerical schemes based on ANOVA-Galerkin projection for stochastic PDEs with large number of random variables. The central idea is to represent the solution using a functional ANOVA decomposition supplemented by appropriate orthogonality constraints so that the weak form can be decoupled into a set of independent low-dimensional subproblems. Numerical studies will be presented for the steady-state and time-dependent stochastic diffusion equation with more than 500 variables.

Prasanth B. Nair
University of Southampton
University of Southampton
pbn@utias.utoronto.ca

Christophe Audouze
The laboratory of signals and systems (L2S)
University Paris-Sud Orsay - CNRS - Supelec
cadouze@gmail.com

CP13
Multilevel Monte Carlo for Uncertainty Quantification in Subsurface Flow

Multilevel Monte Carlo is an efficient variance reduction technique to quantify uncertainties in simulations of subsurface flows with highly varying, rough coefficients, e.g. in radwaste disposal. We study model elliptic problems of single phase flow in random media described by correlated lognormal distributions, discretized in space via (standard and mixed) finite elements. We will demonstrate (theoretically and numerically) significant gains with respect to standard Monte Carlo, leading (in the best case) to an asymptotic cost that is proportional to solving one deterministic PDE.

Robert Scheichl
Department of Mathematical Sciences
University of Bath
masrs@maths.bath.ac.uk

Andrew Cliffe
School of Mathematical Sciences
University of Nottingham
andrew.cliffe@nottingham.ac.uk

Michael B. Giles
Mathematical Institute
Oxford University
Mike.Giles@maths.ox.ac.uk

Minho Park
University of Nottingham
minho.park@nottingham.ac.uk

Aretha Teckentrup, <u>Elisabeth Ullmann</u>
University of Bath
a.l.teckentrup@bath.ac.uk, e.ullmann@bath.ac.uk

CP14
Toward Reduction of Uncertainty in Complex Multi-Reservoir River Systems

Uncertainties are inherent in the operation of any system, however assuming that they are all purely stochastic and independent, both spatially and temporally, may result in unnecessarily large uncertainties that may not be useful for the operation of a system. In this paper we present a novel framework for better modeling uncertainty in complex systems and demonstrate the approach applied to regulated river systems. This framework aims to combine "purely stochastic processes' (not well understood or unpredicted at this stage) with the physical description of the system (e.g., flow dynamics in the case of complex regulated river systems) with the goal of better modeling uncertainties and hence reduce the ranges of the confidence intervals. In this framework, only the stream inflows (external source) are assumed to be purely stochastic. Other uncertain quantities are correlated to the uncertainty of the stream inflows using the dynamics of the river as the physical description of the system. In this framework the dynamics of the river is simulated using the performance graphs approach. For the quantification of uncertainty, rather than doing sampling of the input distributions, we explicitly model the random space (via random variables and processes). We represent uncertainty in stream inflows via an error term modeled as a stochastic process. The resulting system is discretized (in random space) using stochastic collocation, which is distinct from random sampling methods in that the Gaussian nodes are deterministic. By recycling existing deterministic codes, this non-intrusive approach is both more efficient than Monte-Carlo methods and as flexible in their application.

<u>Nathan L. Gibson</u>
Oregon State University
gibsonn@math.oregonstate.edu

Arturo Leon, Christopher Gifford-Miears
School of Civil and Construction Engineering
Oregon State University
arturo.leon@oregonstate.edu, giffordc@onid.orst.edu

CP14
Stochastic Analysis of the Hydrologic Cascade Model, a Polynomial Chaos Approach

In this talk we analyse a Nash cascade of linear reservoirs representing a watershed. It is specified by a system of coupled linear differential equations with random coefficients. A stochastic spectral representation of these parameters is used, together with a polynomial chaos expansion. A system of differential equations is obtained which describe the evolution of the mean and higher-order moments with respect to time.

Franz Konecny
BOKU-University of Natural Resources and Applied
Life Sciences, Vienna
franz.konecny@boku.ac.at

Hans-Peter Nachtnebel
BOKU-University of Natural Resources and Life Sciences,
Vien
hans_peter.nachtnebel@boku.ac.at

CP14
Likelihood-Based Observability Analysis and Confidence Intervals for Model Predictions

Nonlinear dynamic models of biochemical networks contain a large number of parameters. This renders classical approaches for the calculation of confidence regions for parameter estimates and model predictions hardly feasible. We present the so-called prediction profile likelihood which is utilized to generate reliable confidence intervals for model predictions and for a data-based observability analysis. The presented approach constitutes a general concept and is therefore applicable for any kind of prediction model.

<u>Clemens Kreutz</u>
University of Freiburg
Institute of Physics
ckreutz@fdm.uni-freiburg.de

Andreas Raue
Physics Institute, University of Freiburg
andreas.raue@fdm.uni-freiburg.de

Jens Timmer
University of Freiburg
Department of Physics
jeti@fdm.uni-freiburg.de

CP14
Hybrid Stochastic Collocation - Stochastic Perturbation Method for Linear Elastic Problems with Uncertain Material Parameters

We propose a hybrid formulation combining the stochastic collocation (SC) and stochastic perturbation (SP) methods to obtain the response of a linear elastic system with material uncertainties. The material properties are modelled as a memory-less transformation of a Gaussian field, which discretized by a series expansion method. The response of the system is estimated using SC to account for the most important (lower) modes in the series expansion and SP for the other (higher) modes.

<u>Boyan S. Lazarov</u>
Department of Mechanical Engineering
Technical University of Denmark
bsl@mek.dtu.dk

Mattias Schevenels
Department of Civil Engineering, K.U.Leuven
Kasteelpark Arenberg 40, B-3001 Leuven, Belgium
mattias.schevenels@asro.kuleuven.be

CP14
A Comparison Of Uncertainty Quantification Methods Under Practical Industry Requirements

The objective of this paper is to establish comprehensive guidelines for engineers to effectively perform probabilistic design studies through a systematically comparison of uncertainty quantification or probabilistic methods. These methods include 1) Simulation-based approaches such as

Monte Carlo simulation, importance sampling and adaptive sampling, 2) Local expansion-based methods such as Taylor series method or perturbation method, 3) First Order Second Moment (FOSM) based methods, 4) Stochastic expansion-based methods, such as Neumann expansion and polynomial chaos expansion, 5) Numerical integration-based or moments-based methods, such as Point Estimate Method, Eigenvector Dimension Reduction, 6) Regression- or metamodel-based methods, 7) Bayesian methods, and 8) Data classification methods. Both aleatory & epistemic uncertainty will be addressed in the paper. A set of benchmark problems representing different levels of dimensionality, non-linearity and noise level will be used for the comparison.

Liping Wang, Gulshan Singh, Arun Subramaniyan
GE Global Research
wangli@ge.com, singhg@ge.com, subramaa@ge.com

CP15
Rare Events Detection and Analysis of Equity and Commodity High-Frequency Data

We present a methodology to detect unusual trading activity defined as high price movement with relatively little volume traded. The analysis is applied to high-frequency transactions of thousands of equities and the probability of price recovery in the proximity of these rare events is calculated. Similar results are obtained when analyzing commodities with different expiration dates. The propagation of rare events in the commodity structure and the liquidity problems are addressed.

Dragos Bozdog, Ionut Florescu
Stevens Institute of Technology
Department of Mathematical Sciences
dbozdog@stevens.edu, ifloresc@stevens.edu

Khaldoun Khashanah, Jim Wang
Stevens Institute of Technology
Financial Engineering Program
kkhashan@stevens.edu, jwang4@stevens.edu

CP15
Glimpses of Uq, Qmu, and Reliability

We will provide an introduction to quantification of margins and uncertainties (QMU) and reliability. QMU is a summary number that is relatively easy to interpret for decision-making. Reliability is defined as the probability that a given item will perform its intended function for a given period of time under a given set of conditions. The underlying concepts in this definition are probability, intended function, time, and conditions. Reliability is a quantity that can be very difficult to compute for complex systems, and viewed rigorously, is inherently a statistical distribution on the probability of success (or failure) of a system. Both concepts are concerned with uncertainty quantification. We will illustrate with examples from complex systems from our work at Los ALamos National Laboratory.

Aparna V. Huzurbazar, David Collins
Los Alamos National Laboratory
aparna@lanl.gov, dcollins@lanl.gov

CP15
Bayesian Subset Simulation

One of the most important and computationally challenging problems in reliability engineering is to estimate the failure probability of a dynamic system. In cases of practical interest, the failure probability is given by an integral over a high-dimensional uncertain parameter space. Subset Simulation method, provides an efficient algorithm for computing failure probabilities for general high-dimensional reliability problems. In this work, a Bayesian counterpart of the original Subset Simulation method is developed.

Konstantin M. Zuev
Department of Mathematics
University of Southern California
kzuev@usc.edu

James Beck
Division of Engineering and Applied Science
California Institute of Technology
jimbeck@caltech.edu

CP16
Delay in Neuronal Spiking

We study how some delay mechanisms influence interaction between a neuron and its network. Specifically, we look at conduction delay, spike-timing dependent plasticity, and time delay induced by the partial differential equation describing a particular neuron. We further compare the contribution of different delay mechanisms to numerical solutions of the governing cable equation. We study two cases: the case of passive electrical activity and the case of propagating action potential.

Mikhail M. Shvartsman
University of St. Thomas
mmshvartsman@stthomas.edu

CP16
A Gaussian Hierarchical Model for Random Intervals

Many statistical data are imprecise due to factors such as measurement errors, computation errors, and lack of information. In such cases, data are better represented by intervals than single-valued numbers. To model both randomness and imprecision, we propose a Gaussian hierarchical model for random intervals, and develop a minimum contrast estimator that we show is both consistent and asymptotically normal. We extend this model to the time series context and build an interval-valued GARCH model.

Yan Sun
Department of Mathematics & Statistics
Utah State University
yan.sun@usu.edu

Dan Ralescu
Department of Mathematical Sciences
University of Cincinnati
dan.ralescu@uc.edu

CP17
Interval-Based Inverse Problems with Uncertain-

ties

Inverse problems in science and engineering aim at estimating model parameters of a physical system using observations of the models response. However, response measurements are usually associated with uncertainties, and deterministic inverse algorithms hardly provide the associated error estimates for the model parameters. In this work, we will present an interval-based iterative solution that predicts such error exploiting an adjoint -based optimization and the containment-stopping criterion.

Rafi L. Muhanna, Francesco Fedele
Georgia Institute of Technology
rafi.muhanna@gtsav.gatech.edu, fedele@gatech.edu

CP17
Probability Bounds for Nonlinear Finite Element Analysis

A set of possible cumulative probability distributions defined by its bounding functions is one way for representing epistemic and aleatory uncertainty separately. Such sets are known as a probability box (P-box). In this work we will present an interval Monte Carlo method for calculating the non-linear response of structures in terms of P-boxes when system parameters and loading are described as P-boxes. Results obtained show very tight enclosures even for large uncertainties.

Rafi L. Muhanna
Georgia Institute of Technology
rafi.muhanna@gtsav.gatech.edu

Robert Mullen
University of South Carolina
rlm@sc.edu

CP17
A Complete Closed-Form Solution to Stochastic Linear Systems with Fixed Coefficients

Given a fixed but arbitrary coefficient matrix A and a meaningful input probability density d(b) that stochastically describes the other input data b for the system Ax = b, this paper: (1) derives explicit formulas for numerically computing the induced probability that this system has at least one solution x, (2) formulates and then describes the important properties of the optimization problem whose solutions b* (if any) maximize d(b) over all b for which Ax = b has at least one solution x, (3) formulates and then describes the important properties of a general optimization problem whose solutions x* (if any) optimize a given function g(x) over all x for which Ax = b*. This methodology can numerically compete with both the simulation approaches and the simplified deterministic approaches based on expected values and other moment information. In modified form, it might also provide new approaches to systems Ax = b with "fuzzy" data b.

Elmor L. Peterson
Systems Science Consulting
elmor.peterson@gmail.com

CP17
Cramer-Rao Bound for Models of Fat-Water Separation Using Magnetic Resonance Imaging

Magnetic resonance images typically contain both water and fat but most of the information is in the water signal. Different assumptions about the imaging conditions result linear and non-linear models of the image generation. The multiple parameters and non-linearity lead to a version of the Cramer-Rao bound for a parameter if all other parameters were known. We study how the choice in model affects the optimal data acquisition based on minimizing this Cramer-Rao bound.

Angel R. Pineda, Emily Bice
California State University, Fullerton
apineda@fullerton.edu, emily.bice@gmail.com

CP17
Automated Exact Calculation of Test Statistics in Hypothesis Testing

Many classical statistical tests rely on large-sample approximations for determining appropriate critical values. We use a computer algebra system to compute the exact distribution of test statistics under the null hypothesis for the Wilcoxon signed-rank test and the chi-square goodness of fit test, which gives the exact critical value for small sample sizes.

Lawrence Leemis
College of William and Mary
leemis@math.wm.edu

Vincent Yannello
The College of William & Mary
vjyannello@email.wm.edu

CP17
Evidence-Based Approach for the Probabilistic Assessment of Unknown Foundations of Bridges

As of 2005, there were approximately sixty thousand bridges throughout the US identified as having Unknown Foundations. Missing substructure information has made safety monitoring of bridges very difficult for departments of transportation, especially for over-river bridges which are susceptible to scour. An evidence-based methodology is proposed in this paper to determine the unknown characteristics of bridge foundations conditional on information collected from existing bridges. The proposed approach combines the use of a Neural-Network model to compute the foundations bearing capacity, with a Bayesian formulation that allows for defining probability distributions of the foundation type, size and embedment depth, as well as of the soil properties supporting the foundation.

Negin Yousefpour, Zenon Medina Cetina, Jean-Louis Briaud
Texas A&M University
neginyousefpour@gmail.com,   zmedina@civil.tamu.edu,
jbriaud@civil.tamu.edu

CP18
An Approach to Weak Solution Approximation of Stochastic Differential Equations

This paper presents an approach to approximate the weak solution of nonlinear stochastic differential equations. Utilizing the results from the Radon-Nikodym theorem and the Girsanov theorem, the proposed approach introduces a measure transformation so that the Itô process under consideration becomes a Wiener process under the trans-

formed measure. Here we propose the Euler-Maruyama scheme to approximate the stochastic integral involved in calculating the Radon-Nikodym derivative associated with the measure transformation. A detailed analysis of the proposed approximation scheme reveals that the proposed approach is exactly the same as calculating the weak solution using the traditional Euler-Maruyama scheme and thus the proposed approach is weakly convergent with a convergence rate of $\gamma = 1$. A numerical example is presented to validates the proposed approach and illustrate its capability.

Jemin George
U.S. Army Research Laboratory
jemin.george.civ@mail.mil

CP18
Asymptotic Normality and Efficiency for Sobol Index Estimator

In this talk we will study the convergence and the efficiency of Sobol index estimators. More precisely, we will consider the following model

$$Y = f(X, Z)$$

where X and Z are independent random vectors. The importance of each input variable can be measured by $S = \left(\frac{\mathrm{Var}(E(Y|X))}{\mathrm{Var}(Y)}, \frac{\mathrm{Var}(E(Y|Z))}{\mathrm{Var}(Y)} \right)$. We will construct an estimator S_n of S and show that it is asymptotically normal and efficient. At the end of the talk, we will give similar results when f is replaced by some approximation $\tilde{f}$.

Alexandre Janon
LJK / Université Joseph Fourier Grenoble (France)
INRIA Rhône Alpes, France
alexandre.janon@imag.fr

Thierry Klein
Institut de Mathématiques de Toulouse
UMR CNRS 5219 Université de Toulouse
thierry.klein@math.univ-toulouse.fr

Agnes Lagnoux
Institut de Mathématiques de Toulouse UMR CNRS 5219
Universi
lagnoux@univ-tlse2.fr

Maëlle Nodet
Université Joseph Fourier and INRIA, France
maelle.nodet@inria.fr

Clémentine Prieur
LJK / Université Joseph Fourier Grenoble (France)
INRIA Rhône Alpes, France
clementine.prieur@imag.fr

CP18
Frechet Sensitivity Analysis for the Convection-Diffusion Equation

In this work, we consider Frchet derivatives of solutions to the convection-diffusion equation with respect to distributed parameters and demonstrate their applicability in parameter estimation. Under certain conditions, the Frchet derivative operator is Hilbert-Schmidt and thus there are parametric variations that have more impact on the solution than others. These variations can be used

to identify locations for new measurements or data samples. We also analyze an algorithm for approximating these parametric variations.

Vitor Leite Nunes
Interdisciplinary Center for Applied Mathematics,
Virginia Polytechnic Institute & State University
vitor@vt.edu

CP18
Analysis of Quasi-Monte Carlo FE Methods for Elliptic PDEs with Lognormal Random Coefficients

We devise, implement and analyse quasi-Monte Carlo methods for computing the expectations of (nonlinear) functionals of solutions of a class of elliptic partial differential equations with lognormal random coefficients. Our motivation comes from fluid flow in random porous media, where a very large number of random variables is usually needed to give a realistic model of the coefficient field. By using deterministically chosen sample points in an appropriate (usually high-dimensional) parameter space, quasi-Monte Carlo methods can obtain substantially higher convergence rates than classical Monte Carlo. An analysis in appropriate function spaces confirms this also theoretically. The analysis is particularly challenging since in the lognormal case the PDE is neither uniformly elliptic nor uniformly bounded and the parametrisation of the coefficient is nonlinear.

Robert Scheichl
Department of Mathematical Sciences
University of Bath
masrs@maths.bath.ac.uk

Ivan G. Graham
University of Bath
I.G.Graham@bath.ac.uk

Frances Y. Kuo
School of Mathematics and Statistics
University of New South Wales
f.kuo@unsw.edu.au

James Nichols
University of New South Wales, Sydney
james.ashton.nichols@gmail.com

Christoph Schwab
ETH Zuerich
SAM
christoph.schwab@sam.math.ethz.ch

Ian H. Sloan
University of New South Wales
School of Mathematics
i.sloan@unsw.edu.au

CP19
Maximum Entropy Construction for Data-Driven Analysis of Diffusion on Random Manifolds

A data-driven approach is developed for the diffusion on manifolds with unknown geometry. Given limited number of samples drawn from the manifold, our objective is to characterize the geometry, while accounting for inevitable uncertainties due to measurement noise and scarcity of samples. We will present a MaxEnt construction for un-

certainty representation of the graph Laplacian used to approximate the Laplace-Beltrami operator. We also discuss the adaptation of this formulation for information diffusion in social networks.

Hadi Meidani
University of Southern California
meidani@usc.edu

Roger Ghanem
University of Southern California
Aerospace and Mechanical Engineering and Civil
Engineering
ghanem@usc.edu

CP19
Multiple Signal Classification in Covariance Space of EEG Data

The objective is to find discriminative features in the EEG signals to mark various stages of drowsiness in vehicle operators. Existing methods are only able to distinguish between extreme stages. In this research, we are trying to use metrics on the covariance space of EEG data to identify the evolution of the state of fatigue from low to high. We have conducted experiments to induce continuous fatigue in human subjects while keeping them awake for about 36 hours. The EEG data has been recorded over 3-hours interval. Eventually we intend to build a spatio-temporal model of evolution of fatigue in the covariance space of EEG data.

Deepashree Sengupta
Indian Institute of Technology, Kharagpur
deepashreesengupta@gmail.com

Aurobinda Routray
Professor, Department of Electrical Engineering
Indian Institute of Technology, Kharagpur
aroutray@ee.iitkgp.ernet.in

CP19
Dynamic Large Spatial Covariance Matrix Estimation in Application to Semiparametric Model Construction Via Variable Clustering: the Sce Approach

We consider estimating a large spatial covariance matrix of the high-dimensional time series by thresholding, quantify the interplay between the spatial estimators' consistency and the temporal dependence level, and prove a CV result for threshold selection. Given a consistently estimated matrix and its natural links with semiparametrics, we screen, cluster the explanatory variables and construct the corresponding semiparametric model to be further estimated with sign constraints. We call this the SCE approach.

Song Song
University of California, Berkeley
ssoonngg123@gmail.com

CP19
Random Matrix Based Approach for Adaptive Estimation of Covariance Matrix

The work considers the problem of estimating unknown covariance matrix, $\mathbf{Q}$, of process noise in linear dynamic system based on corrupted state measurements data. Here, $\mathbf{Q}$ is *directly* treated as a symmetric, positive-definite random matrix unlike other approaches where each element of $\mathbf{Q}$ is treated as random variable or $\mathbf{Q}$ is itself parameterized by a set of scalar-valued random variables. The probability density function (pdf) of $\mathbf{Q}$ is estimated by employing maximum entropy principle. The theory of multiple model and Kalman Filter are then used to update this pdf over time, resulting in a pdf with sharp peak around the true covariance matrix once sufficient number of measurements are made.

Sonjoy Das, Sonjoy Das, Kumar Vishwajeet
University at Buffalo
sonjoy@buffalo.edu, sonjoy@buffalo.edu,
kumarvis@buffalo.edu

Puneet Singla
Mechanical & Aerospace Engineering
University at Buffalo
p.singla@gmail.com

CP20
Determining Critical Parameters of Sine-Gordon and Nonlinear Schrödinger Equations with a Point-Like Potential Using Generalized Polynomial Chaos Methods

We consider the sine-Gordon and nonlinear Schrödinger equations with a point-like singular source term. The soliton interaction with such a singular potential yields a critical solution behavior. That is, for the given value of the potential strength or the soliton amplitude, there exists a critical velocity of the initial soliton solution, around which the solution is either trapped by or transmitted through the potential. In this talk, we propose an efficient method for finding such a critical velocity by using the generalized polynomial chaos (gPC) method. For the proposed method, we assume that the soliton velocity is a random variable and expand the solution in the random space using the orthogonal polynomials. We consider the Legendre and Hermite chaos with both the Galerkin and collocation formulations. The proposed method finds the critical velocity accurately with spectral convergence. Thus the computational complexity is much reduced. The very core of the proposed method lies in using the mean solution instead of reconstructing the solution. The mean solution converges exponentially while the gPC reconstruction may fail to converge to the right solution due to the Gibbs phenomenon in the random space. Numerical results confirm the accuracy and spectral convergence of the method.

Debananda Chakraborty
Ph.D. student
dc58@buffalo.edu

Jae-Hun Jung
Department of Mathematics
SUNY at Buffalo
jaehun@buffalo.edu

CP20
A Comparison of Dimensionality Reduction Techniques in Scientific Applications

High-dimensional data sets, where each data item is represented by many attributes or features, are a challenge in data mining. Irrelevant attributes can reduce the accuracy of classification algorithms, while distance-based clustering algorithms suffer from a loss of meaning of the term

"nearest neighbors". Using data sets from scientific applications, we present a comparison of different dimensionality reduction methods, including various feature selection techniques, as well as linear and non-linear feature transform methods.

Ya Ju Fan, Chandrika Kamath
Lawrence Livermore National Laboratory
fan4@llnl.gov, kamath2@llnl.gov

CP20
Computational Methods for Statistical Learning Using Support Vector Machine Classifiers

An augmented Lagrangian algorithm for solving equality and bound constrained quadratic problems will be presented for use in support vector machine (SVM) classification. Examples will include images and a diabetes data set. The algorithm will be compared with existing optimization techniques and the SVM method will be compared with quadratic discriminant analysis, as well as a general linearized model for the diabetes data set.

Marylesa Howard
The University of Montana
marylesa.howard@umontana.edu

CP20
A Hidden Deterministic Solution to the Quantum Measurement Problem

In this paper we present a nonconventional method of establishing a hidden but computationally realizable deterministic solution to quantum measurement problems in the non-infinite, non-zero quantized energy limits. Our approach is not in contradiction with Heisenberg's Uncertainty Principle, rather it determines energy (E) and momentum (p) of a quantum particle as functions of uncertainties,viz $E = f(\Delta E)$ and $p = f(\Delta p)$. Thus an observer gets $E \pm \triangle E$ and $p \pm \triangle p$ as the observed values of the energy and momentum of the said particle.

Pabitra Pal Choudhury
Professor in Applied Statistics Unit, ISI Kolkata 700108
pabitra@isical.ac.in; pabitrapalchoudhury@gmail.co

Swapan Kumar Dutta
Retired Scientist
pabitrapalchoudhury@gmail.com

MS1
Super-parameterisation of Oceanic Deep Convection using Emulators

Misrepresentation of sub-grid scale processes can increase the uncertainty in the results of large scale models. Despite the existence of detailed numerical models that resolve sub-grid scale processes, embedding these in a large scale model is often computationally prohibitive. A viable alternative is to encapsulate our knowledge about the sub-grid scale model in an emulator and use this as a surrogate. We apply this paradigm of 'super-parameterisation' to an oceanic deep convection problem.

Yiannis Andrianakis
National Oceanography Centre
University of Southampton, UK
i.andrianakis@soton.ac.uk

MS1
Effective and Efficient Handling of Ill-Conditioned Correlation Matrices in Kriging and Gradient Enhanced Kriging Emulators through Pivoted Cholesky Factorization

Kriging or Gaussian Process emulators are popular because they interpolate build data if the correlation matrix is R.S.P.D. and produce a spatially varying error estimate. However, handling ill-conditioned correlation matrices can be challenging. The rows/columns of an ill-conditioned matrix substantially duplicate information. Pivoted Cholesky ranks points by their new information content; then low information points are discarded. Since discarded points contain the least new information, they best remediate ill-conditioning and are the easiest to predict.

Keith Dalbey
Sandia National Laboratories
kdalbey@sandia.gov

MS1
History Matching: An alternative to Calibration for a Galaxy Formation Simulation

In the context of computer models, calibration is a vital technique whereby an emulator is used to obtain a posterior distribution over the input space of the computer simulator. However, this process can be extremely challenging. We discuss a powerful alternative known as history matching that can either serve as a prelude to a full calibration to greatly improve efficiency, or that can in several cases replace calibration entirely. Work from Mitchell Prize winning paper.

Ian Vernon
University of Durham, UK
i.r.vernon@durham.ac.uk

MS1
Emulation of Count Data in Healthcare Models

Natural History Models are simulators used in healthcare applications to simulate patients' outcomes from certain illnesses. Their output is typically count data and for rare illnesses zeros are common. The simulators rely on many unknown parameters, but calibration using Monte Carlo methods is impractical due to computational expense. Instead we calibrate using an emulator as a surrogate for the simulator, showing how appropriate regions of parameter space are identified for the emulator to perform well.

Ben Youngman
University of Sheffield, UK
b.youngman@sheffield.ac.uk

MS2
Bayesian Inference with Optimal Maps

We present a new approach to Bayesian inference that entirely avoids Markov chain simulation, by constructing a map that *pushes forward* the prior measure to the posterior measure. Existence and uniqueness of a suitable measure-preserving map are established by formulating the problem in the context of optimal transport theory. We discuss various means of explicitly parameterizing the map and computing it efficiently through solution of a stochastic optimization problem, exploiting gradient information

from the forward model. The resulting algorithm overcomes many of the computational bottlenecks associated with Markov chain Monte Carlo. Advantages of a map-based representation of the posterior include analytical expressions for posterior moments and the ability to generate arbitrary numbers of independent posterior samples without additional likelihood evaluations or forward solves. The optimization approach also provides clear convergence criteria for posterior approximation and facilitates model selection through automatic evaluation of the marginal likelihood. We demonstrate the accuracy and efficiency of the approach on nonlinear inverse problems of varying dimension, involving the inference of parameters appearing in ordinary and partial differential equations.

Tarek El Moselhy, Youssef M. Marzouk
Massachusetts Institute of Technology
tmoselhy@mit.edu, ymarz@mit.edu

MS2
Sample-based UQ via Computational Linear Algebra (Not MCMC)

Sample-based inverse and predictive UQ has proven effective, though MCMC sampling is expensive. Several groups are now developing links between computational linear algebra and sampling algorithms with the aim of reducing the cost of sampling. Currently these links are exact for Gaussian distributions, only, but do indicate how the more general case should look.

Colin Fox
University of Otago, New Zealand
fox@physics.otago.ac.nz

MS2
Toward Extreme-scale Stochastic Inversion

We are interested in inferring earth models from global seismic wave propagation waveforms. This inverse problem is most naturally cast as a large-scale statistical inverse wave propagation problem in the framework of Bayesian inference. The complicating factors are the high-dimensional parameter spaces (due to discretization of infinite-dimensional parameter fields) and very expensive forward problems (in the form of 3D elastic-acoustic coupled wave propagation PDEs). Here we present a so-called stochastic Newton method in which MCMC is accelerated by constructing and sampling from a proposal density that builds a local Gaussian approximation based on local gradient and Hessian (of the log posterior) information. Hessian manipulations (inverse, square root) are made tractable by a low rank approximation that exploits the compact nature of the data misfit operator. This amounts to a reduced model of the parameter-to-observable map. We apply the method to 3D seismic inverse problems with several million parameters, illustrating the efficacy and scalability of the low rank approximation.

Tan Bui
University of Texas at Austin
tanbui@ices.utexas.edu

Carsten Burstedde
Institut fuer Numerische Simulation
Universitaet Bonn
burstedde@ins.uni-bonn.de

Omar Ghattas

University of Texas at Austin
omar@ices.utexas.edu

James R. Martin
University of Texas at Austin
Institute for Computational Engineering and Sciences
jmartin@ices.utexas.edu

Georg Stadler
University of Texas at Austin
georgst@ices.utexas.edu

Lucas Wilcox
HyPerComp
me@lucaswilcox.com

MS2
Nonparametric Bayesian Inference for Inverse Problems

I will consider the Bayesian approach to inverse problems in the setting where Gaussian random field priors are adopted. I will study random walk type Metropolis algorithms and demonstrate how small modifications in the standard algorithm can lead to an order of magnitude speed up, in terms of the size of the discretization used.

Andrew Stuart
Mathematics Institute,
University of Warwick
a.m.stuart@warwick.ac.uk

MS3
Global Sensitivity Analysis with Correlated Inputs: Numerical Aspects in Distribution-Based Sensitivity Measures

In this work, we address the sensitivity of model output utilizing density-based importance measures and a recently introduced sensitivity measures based on repeated Kolmogorov-Smirnov Test. We offer a comparison of the two statistics which, as we are to see, are closely related. We show that they hare closely related. We then show that they can be estimated from given samples. We use this fact to study their estimation in the presence of correlations. Numerical results for examples in which the analytical solution is known are discussed.

Emanuele Borgonovo
Bocconi University (Milan)
ELEUSI Research Center
emanuele.borgonovo@unibocconi.it

MS3
Sensitivity Indices Based on a Generalized Functional ANOVA

Functional ANOVA allows defining variance based sensitivity indices of any order in the case of independent inputs. Under a dependence-type condition on the joint inputs distribution, we derive a generalization of Hoeffding decomposition, from which we introduce sensitivity indices of any order even for correlated inputs. We also propose an algorithm to compute these indices in the particular case where inputs are correlated two by two.

Clémentine Prieur
LJK / Université Joseph Fourier Grenoble (France)

INRIA Rhône Alpes, France
clementine.prieur@imag.fr

Gaelle Chastiang
Project-Team INRIA MOISE
Grenoble
gaelle.chastaing@imag.fr

Fabrice Gamboa
Laboratory of Statistics and Probability
University of Toulouse
fabrice.gamboa@math.univ-toulouse.fr

MS3

Global Sensitivity Analysis for Systems with Independent and/or Correlated Inputs

Structural and Correlative Sensitivity Analysis (SCSA) provides a new unified framework of global sensitivity analysis for systems with independent and correlated variables based on a covariance decomposition of the output variance. Three sensitivity indices were defined to give a full description, respectively, of the total, structural and correlative contributions of the inputs upon the output. For independent inputs, these indices reduce to a single index consistent with the variance-based method as a special case of the new treatment.

Herschel Rabitz
Department of Chemistry
Princeton University
hrabitz@Princeton.EDU

Genyuan Li
Princeton University
genyuan_li@yahoo.com

MS3

Variance-based Sensitivity Indices for Models with Correlated Inputs Using Polynomial Chaos Expansions

The variance decomposition techniques used for global sensitivity analysis are well established as a means for quantifying the uncertainty of the output of a computer model that may be attributed to each input parameter. The classical framework only holds for independent input parameters. In this paper the covariance decomposition proposed by Rabitz is adapted to polynomial chaos expansions of the model response in order to estimate the structural and correlative importance of each input parameter.

Bruno Sudret
Université Paris-Est
Laboratoire Navier
bruno.sudret@enpc.fr

Yann Caniou, Alexandre Micol
Phimeca
caniou@phimeca.com, amicol@phimeca.com

MS4

Quantifying and Reducing Uncertainties on a Set of Failure Using Random Set Theory and Kriging

In computer-assisted robust design and safety studies, calculating probability of failures based on approximation models of the objective function is a problem of growing interest, and has recently inspired several strategies relying on Kriging (e.g., Stepwise Uncertainty Reduction strategies). An even more challenging problem is to describe the set of all dangerous configurations, i.e. the set of input parameters such the output of interest exceeds a given threshold T. Mathematically, if f is the response, such set of failure is denoted by $G = \{x : f(x) \geq T\}$. Estimating G in a severely limited budget of evaluations of f is a difficult problem, and a suitable use of Kriging may help solving it in practice. Starting from an initial set of evaluations of f at an initial Design of Experiments, one can indeed calculate coverage probabilities and/or simulate Gaussian Field realizations conditionally on the available information. We propose to use such notions to sum up the current knowledge on the excursion set, and also to define new SUR strategies based on decreasing some measure of variability of the excursion set distribution. We recently revisited classical notions of random set theory to obtain candidate "expectations' for random sets of excursion, as well as candidate quantifications of uncertainty related to the investigated expectation notions. In this talk we focus on the so called Vorob'ev expectation (for which there is a candidate quantification of uncertainty naturally associated) and derive a new SUR sampling criterion associated to this uncertainty. Implementation issues are discussed and the criterion is illustrated on mono and multi-dimensional examples.

Chevalier Clément
IRSN and UNIBE
clement.chevalier@irsn.fr

David Ginsbourger
Department of Mathematics and Statistics, University of Bern
david.ginsbourger@stat.unibe.ch

Julien Bect
SUPELEC, Gif-sur-Yvette, France
julien.bect@supelec.fr

Ilya Molchanov
Department of Mathematics and Statistics
University of Bern
ilya@stat.unibe.ch

MS4

Sampling Strategy for Stochastic Simulators with Heterogeneous Noise

Kriging-based approximation is a useful tool to approximate the output of a Monte-Carlo simulator. Such simulator has the particularity to have a known relation between its accuracy and its computational cost. Our objective is to find a sampling strategy optimizing the tradeoff between the fidelity and the number of simulation given a limited computational budget when the fidelity of the M-C simulator depends on the value of the input space parameter. The presented strategies are illustrated on an industrial example of neutron transport code.

Loic Le Gratiet
CEA, DAM, DIF
loic.le-gratiet@cea.fr

Josselin Garnier
Universite Paris 7
garnier@math.jussieu.fr

MS4
Optimization of Expensive Computer Experiments Using Partially Converged Simulations and Space-time Gaussian Processes

To alleviate the cost of numerical experiments, it is sometimes possible to stop at early stage the convergence of a simulation and exploit the obtained response, the gain in time being at the price of convergence error. We propose to model such data using a GP model in the joint space of design parameters and computational time, and perform optimization using an EGO-like strategy with the help of a new statistic: the Expected Quantile Improvement.

Victor Picheny
European Center for Research and Advanced Training in Scient
picheny@cerfacs.fr

MS4
Models with Complex Uncertain Inputs

We consider the problem of investigating the consequences of an event that releases contamination into the atmosphere. Simulators for such events depend on atmospheric and meteorological conditions over at least a six-hour time span. For example, wind strength and direction will be influential in assessing the severity of contamination across a spatial window. The common strategy for simulating these conditions is to sample observed stretches of data. We consider how to generate an informative sample and how to carry out the subsequent analysis.

David M. Steinberg
Tel Aviv University
dms@post.tau.ac.il

MS5
Approximation and Error Estimation in High Dimensional Stochastic Collocation Methods on Arbitrary Sparse Samples

Stochastic collocation methods are an attractive choice to characterize uncertainty because of their non-intrusive nature. High dimensional stochastic spaces can be approximated well for smooth functions with sparse grids. There has been a focus in extending this approach to non-smooth functions using adaptive sparse grids. This presentation will present both adaptive approximation methods and error estimation techniques for high dimension functions.

Rick Archibald
Computational Mathematics Group
Oak Ridge National Labratory
archibaldrk@ornl.gov

MS5
Spatially Varying Stochastic Expansions for Embedded Uncertainty Quantification

Existing discretizations for stochastic PDEs, based on a tensor product between the deterministic basis and the stochastic basis, treat the required resolution of uncertainty as uniform across the physical domain. However, solutions to many PDEs of interest exhibit spatially localized features that may result in uncertainty being severely over or under-resolved by existing discretizations. In this talk, we explore the mechanics and accuracy of using a spatially varying stochastic expansion. This is achieved through an adaptive refinement algorithm where simple error estimates are used to independently drive refinement of the stochastic basis at each point in the physical domain. Results will be presented comparing the performance of this method with other embedded UQ techniques.

Eric C. Cyr
Scalable Algorithms Department
Sandia National Laboratotories
eccyr@sandia.gov

MS5
Simultaneous Local and Dimension Adaptive Sparse Grids for Uncertainty Quantification

Polynomial methods, such as Polynomial Chaos, are often used to construct surrogates of expensive numerical models. When the response surface is smooth these techniques accurately reproduce the model variance. However when discontinuities are present or local metrics, such as probability of failure, are of interest the utility of these methods decreases. Here we propose a greedy, locally and dimension adaptive sparse grid interpolation method which restricts function evaluations to dimensions and regions of interest. The adaptivity is guided by a weighted local interpolation error estimate. The proposed method is highly efficient when only a sub-region of a high-dimensional input space is important.

John D. Jakeman
Sandia National Labs
jdjakem@sandia.gov

Stephen G. Roberts
Australian National University
stephen.roberts@anu.edu.au

MS5
A Posteriori Error Analysis and Adaptive Sampling for Probabilities using Surrogate Models

Surrogate methods have grown in popularity in recent years for stochastic differential equations due to their high-order convergence rates for moments of the solution. Oftentimes, however, the objective is to compute probabilities of certain events, which is performed by sampling the surrogate model. Unfortunately, each of these samples contains discretization error which affects the reliability. We apply adjoint techniques to quantify the accuracy of statistical quantities by estimating the error in each sample and seek to improve the surrogate model through drive adaptive refinement.

Tim Wildey
Sandia National Laboratory
tmwilde@sandia.gov

Troy Butler
Institute for Computational Engineering and Sciences
University of Texas at Austin
tbutler@ices.utexas.edu

MS6
Heat Kernel Smoothing on an Arbitrary Manifold Using the Laplace-Beltrami Eigenfunctions

We present a novel kernel smoothing framework on curved surfaces using the Laplace-Beltrami eigenfunctions. The

Green's function of an isotropic diffusion equation is analytically represented using the Laplace-Beltrami eigenfunctions. The Green's function is then used in explicitly constructing heat kernel smoothing as a series expansion. Our analytic approach offers many advantages over previous filtering methods that directly solve diffusion equations using FEM. The method is illustrated with various surfaces obtained from medical images.

Moo Chung
Department of Biostatistics and Medical Informatics
University of Wisconsin-Madison
mkchung@wisc.edu

MS6
Sparse Grids for Regression

We consider the sparse grid combination technique for regression, which we regard as a problem of function reconstruction in some given function space. We use a regularised least squares approach, discretised by sparse grids and solved using the so-called combination technique, where a certain sequence of conventional grids is employed. The sparse grid solution is then obtained by the addition of these partial solutions with certain predefined combination coefficients. We show why the original combination technique is not guaranteed to converge with higher discretisation levels in this setting, but that a so-called optimised combination technique can be used instead.

Jochen Garcke
University of Bonn
garcke@ins.uni-bonn.de

MS6
Second-Order Comparison of Random Functions

Given two samples of random square-integrable functions, we consider the problem of testing whether they share the same second-order structure. Our study is motivated by the problem of determining whether the mechanical properties of short DNA loops are significantly affected by their base-pair sequence. The testing problem is seen to involve aspects of ill-posed inverse problems and a test based on a Karhunen-Love approximation of the Hilbert-Schmidt distance of the empirical covariance operators is proposed and investigated. More generally, we develop the notion of a dispersion operator and construct a family of tests. Our procedures are applied to a sample of DNA minicircles obtained via the electron microscope.

Victor M. Panaretos
Section de Mathématiques
EPFL
victor.panaretos@epfl.ch

MS6
Spatial Spline Regression Models

We deal with the problem of surface estimation over irregularly shaped domains, featuring complex boundaries, strong concavities and interior holes. Adopting an approach typical of Functional Data Analysis, we propose a Spatial Spline Regression model that efficiently handle this problem; the model also accounts for covariate information, can comply with general conditions at the domain boundary and has the capacity to incorporate a priori information about the surface shape.

Laura M. Sangalli
MOX Department of Mathematics
Politecnico Milano, Italy
laura.sangalli@polimi.it

Laura Azzimonti
MOX Department of Mathematics
Politecnico di Milano, Italy
laura.azzimonti@mail.polimi.it

James O. Ramsay
McGill University, Montreal, Canada
ramsay@psych.mcgill.ca

Piercesare Secchi
MOX - Department of Mathematics
Politecnico di Milano, ITALY
piercesare.secchi@polimi.it

MS7
Global Sensitivity and Reduction of Very High-Dimensional Models with Correlated Inputs

Models originating from observed data or from computer code can be very high-dimensional. Total contribution from model input X_i to variance of model output Y is defined as $V_{T_i} = \text{Var}(Y) - \text{Var}[E(Y|\mathbf{X}_{-i})]$, where $\mathbf{X}_{-i}$ corresponds to all inputs except X_i. We develop an efficient algorithm to compute V_{T_i} for models with thousands of possibly correlated inputs with arbitrary distributions. The number of required model samples is independent of the number of inputs. The resulting global sensitivities $V_{T_i}/\text{Var}(Y)$ can be used to create a reduced model for fast output prediction and uncertainty quantification. The developed algorithms are implemented in our software Go-SUM (Global Optimizations, Sensitivity and Uncertainty in Models).

Vladimir Fonoberov
Chief Scientist
AIMdyn, Inc
vfonoberov@aimdyn.com

Igor Mezic
University of California, Santa Barbara
mezic@engineering.ucsb.edu

MS7
Uncertainty Quantification in Energy Efficient Building Retrofit Design

One area of engineering where uncertainty quantification and mitigation is not only desired, but actually necessary is energy efficient building retrofit design. Buildings are complex systems with large number of parameters that are often not properly measured and recorded (e.g. equipment efficiencies) or that have inherently large uncertainties associated with them (e.g. occupancy patterns). In this talk we discuss mathematical methods and technical challenges involved with UQ for retrofit design.

Slaven Peles
United Technologies Research Center
PelesS@utrc.utc.com

MS7
Iterative Methods for Propagating Uncertainty through Networks of Switching Dynamical Systems

Networks of switching dynamical systems arise naturally in a vast variety of applications. These systems can be challenging for analysis due to non-smooth dynamics. Here, we develop methods to perform uncertainty quantification on switching systems using polynomial chaos based on wavelet expansions. Since the number of equations required scales exponentially, we develop novel iterative methods to simulate networks of switching dynamical systems. We demonstrate these methods on a large network of switching oscillators.

Tuhin Sahai
United Technologies
sahait@utrc.utc.com

MS7
NIPC: A MATLAB GUI for Wider Usability of Nonintrusive Polynomial Chaos

Polynomial Chaos theory is a sophisticated method for a fast stochastic analysis of dynamic systems with few random parameters. Classically, all system laws are reformulated into deterministic equations, but recently, a nonintrusive variation has been developed for application with black boxes. After a brief introduction of this concept, we would like to present a tool which makes the numerous adjustments and the understanding of the advanced mathematical roots of Polynomial Chaos irrelevant for the user.

Kanali Togawa
E.ON Energy Research Center - RWTH
Aachen University
ktogawa@eonerc.rwth-aachen.de

Antonello Monti
E.ON Energy Research Center - RWTH Aachen
University
amonti@eonerc.rwth-aachen.de

MS8
Speeding up the Sensitivity Analysis of an Epidemiological Model

This presentation describes a probabilistic sensitivity analysis of an epidemiological simulator of rotavirus. We used both advanced input screening techniques and emulator-based methods to make the process more efficient and focussed on the relevant regions of the input space. The key to successfully applying these methods was the quantification of expert uncertainty about the input parameters. The methods for expert elicitation will be described and their use in the sensitivity analysis will be illustrated.

John Paul Gosling
University of Leeds
j.p.gosling@leeds.ac.uk

MS8
Sensitivity Analysis of a Global Aerosol Model to Quantify the Effect of Uncertain Model Parameters

We present a sensitivity analysis of a global aerosol model using Gaussian process emulation. We present results for the sensitivity of global cloud condensation nuclei to 37 uncertain process parameters and emissions. We show global maps of the total uncertainty in several aerosol quantities as well as a breakdown of the main factors controlling the uncertainty. These results provide a very clear guide for the reduction in model uncertainty through targeted model development.

Lindsay Lee, Kenneth Carslaw, Kirsty Pringle
University of Leeds
l.a.lee@leeds.ac.uk,   k.s.carslaw@leeds.ac.uk,
k.pringle@leeds.ac.uk

MS8
Sensitivity Analysis for Complex Computer Models

We discuss the problem of quantifying the importance of uncertain input parameters in a computer model; which input parameters should we learn about to best reduce output uncertainty? Two standard tools are reviewed: variance-based sensitivity analysis, and decision theoretic measures based on the value of information. For computationally expensive models, computational methods are presented for calculating these measures using Gaussian-process surrogate models. These tools will be applied in the remaining three talks.

Jeremy Oakley
University of Sheffield
j.oakley@sheffield.ac.uk

MS8
Managing Model Uncertainty in Health Economic Decision Models

Health economic models predict the costs and health effects associated with competing decision options (e.g. recommend drug X versus Y). Current practice is to quantify input uncertainty, but to ignore uncertainty due to deficiencies in model structure. Given a relatively simple but imperfect model, is there value in incorporating additional complexity to better describe the decision problem? We derive the 'expected value of model improvement' via a decision theoretic sensitivity analysis of model discrepancy.

Mark Strong, Jeremy Oakley
University of Sheffield
m.strong@sheffield.ac.uk, j.oakley@sheffield.ac.uk

MS9
Hybrid UQ Method for Multi-Species Reactive Transport

Uncertainty quantification (UQ) for multi-physics applications is challenging for both intrusive and non-intrusive methods. A question naturally arises: Can we take the best of both worlds to introduce a 'hybrid' UQ methodology for multi-physics applications? This minisymposium brings together researchers who are exploring hybrid UQ methods. In particular, we emphasize techniques that propagate global uncertainties yet allow individual physics components to use their local intrusive or non-intrusive UQ methods. Relevant issues for discussions are: hybrid uncertainty propagation algorithms, dimension reduction, Bayesian data fusion techniques, design of hybrid computational framework, and scalable algorithms for hybrid UQ.

Xiao Chen

Lawrence Livermore National Laboratory
Center for Applied Scientific Computing
chen73@llnl.gov

Brenda Ng, Yunwei Sun, Charles Tong
Lawrence Livermore National Laboratory
ng30@llnl.gov, sun4@llnl.gov, tong10@llnl.gov

MS9

Preconditioners/Multigrid for Stochastic Polynomial Chaos Formulations of the Diffusion Equation

This talk presents (parallel) preconditioners and multigrid solvers for solving linear systems of equations arising from stochastic polynomial chaos (PC) formulations of the diffusion equation with random coefficients. These preconditioners/solvers are an extension of the preconditioner developed in [**?**] for strongly coupled systems of elliptic partial equations that are norm equivalent to systems that can be factored into an algebraic coupling component and a diagonal differential component, as is the case for the systems produced by PC formulations of the diffusion equation.

Barry Lee
Pacific Northwest National Laboratory
Barry.Lee@pnnl.gov

MS9

A High Performance Hybrid pce Framework for High Dimensional UQ Problems

In the domain of stochastic multi-physics problems, traditional non-intrusive and intrusive UQ methods are expensive and preclude a much-needed modular plug and play solver infrastructure. We present a hybrid UQ methodology to tackle these challenges. A conditional polynomial representation of the stochastic solution vector is used to track local and global uncertainty propagation between modules. The frameworks parallel efficiency and spectral accuracy is shown using a multi-species reaction-flow problem modeled as a non-linear PDE system.

Akshay Mittal
Department of Mathematics
Stanford University
mittal0@stanford.edu

MS9

Stochastic Dimension Reduction Techniques for Uncertainty Quantification of Multiphysics Systems

Uncertainty quantification of multiphysics systems represents numerous mathematical and computational challenges. Indeed, uncertainties that arise in each physics in a fully coupled system must be captured throughout the whole system, the so-called curse of dimensionality. We present techniques for mitigating the curse of dimensionality in network-coupled multiphysics systems by using the structure of the network to transform uncertainty representations as they pass between components. Examples from the simulation of nuclear power plants will be discussed.

Eric Phipps
Sandia National Laboratories
Optimization and Uncertainty Quantification Department
etphipp@sandia.gov

Maarten Arnst
Universite' de Liege
maarten.arnst@ulg.ac.be

Paul Constantine
Sandia National Labs
paul.g.constantine@gmail.com

Roger Ghanem
University of Southern California
Aerospace and Mechanical Engineering and Civil Engineering
ghanem@usc.edu

John Red-Horse
Validation and Uncertainty Quantification Processes
Sandia National Laboratories
jrredho@sandia.gov

Tim Wildey
Sandia National Laboratory
tmwilde@sandia.gov

MS10

First Order k-th Moment Finite Element Analysis of Nonlinear Operator Equations with Stochastic Data

We develop and analyze a class of efficient algorithms for uncertainty quantification of nonlinear operator equations. The algorithms are based on sparse Galerkin discretizations of tensorized linearizations at nominal parameters. Specifically, we analyze a class of abstract nonlinear, parametric operator equations

$$J(\alpha, u) = 0$$

for random parameters α with realizations in a neighborhood of a nominal parameter α_0. Under some structural assumptions on the parameter dependence, random parameters $\alpha(\omega) = \alpha_0 + r(\omega)$ are shown to imply a unique random solution $u(\omega) = S(\alpha(\omega))$. We derive an operator equation for the deterministic computation of k-th order statistical moments of the solution fluctuations $u(\omega) - S(\alpha_0)$, provided that statistical moments of the random parameter perturbation $r(\omega)$ are known. This formulation is based on the linearization in a neighborhood of a nominal parameter α_0. We provide precise bounds for the linearization error by means of a Newton-Kantorovich-type theorem. We present a sparse tensor Galerkin discretization for the tensorized first order perturbation equation and deduce that sparse tensor Galerkin discretizations of this equation converge in accuracy vs. complexity which equals, up to logarithmic terms, that of the Galerkin discretization of a single instance of the mean field problem.

Alexey Chernov
University of Bonn
chernov@hcm.uni-bonn.de

Christoph Schwab
ETH Zuerich
SAM
christoph.schwab@sam.math.ethz.ch

MS10

An Adaptive Iterative Method for

High-dimensional Stochastic PDEs

A new approach for constructing low-rank solutions to stochastic partial differential equations is presented. Our algorithm exploits the notion that the stochastic solution and functionals thereof may live on low-dimensional manifolds, even in problems with high-dimensional stochastic inputs. We use residuals of the stochastic PDE to sequentially and adaptively build bases for both the random and deterministic components of the solution. By tracking the norm of the residual, meaningful error measures are provided to determine the quality of the solution. The approach is demonstrated on Maxwell's equations with uncertain boundaries and on linear/nonlinear diffusion equations with log-normal coefficients, characterized by several hundred input dimensions. In these problems, we observe order-of-magnitude reductions in computational time and memory compared to many state-of-the-art intrusive and non-intrusive methods.

Tarek El Moselhy, Youssef M. Marzouk
Massachusetts Institute of Technology
tmoselhy@mit.edu, ymarz@mit.edu

MS10
Adjoint Enhancement Within Global Stochastic Methods

This presentation will explore the use of local adjoint sensitivities within global stochastic approximation methods for the purposes of improving the scalability of uncertainty quantification methods with respect to random dimension. Methodologies of interest include generalized polynomial chaos, based on regression over unstructured grids; stochastic collocation, based on gradient-enhanced interpolation polynomials on structured grids; and global reliability methods, using gradient-enhanced kriging on unstructured grids. Efficacy of these gradient-enhanced approaches will be assessed based on relative efficiency (speed-up with adjoint gradient inclusion) and numerical robustness (ill-conditioning of solution or basis generation).

Michael S. Eldred
Sandia National Laboratories
Optimization and Uncertainty Quantification Dept.
mseldre@sandia.gov

Eric Phipps
Sandia National Laboratories
Optimization and Uncertainty Quantification Department
etphipp@sandia.gov

Keith Dalbey
Sandia National Laboratories
kdalbey@sandia.gov

MS10
Stochastic Collocation Methods in Unstructured Grids

We present a framework for stochastic collocation method on arbitrary grids. The method utilizes a newly developed least orthogonal interpolation theory to construct high-order polynomial approximations of the stochastic solution, based on the collocation results of any type of grids in arbitrary dimensions. We present both the mathematical theory and numerical implementation. Examples are provided to demonstrate the flexibility of the methods.

Akil Narayan, Dongbin Xiu
Purdue University
akil@purdue.edu, dxiu@purdue.edu

MS11
A Dynamic Programming Approach to Sequential and Nonlinear Bayesian Experimental Design

We present a framework for optimal sequential Bayesian experimental design, using information theoretic objectives. In particular, we adopt a "closed-loop" approach that uses the results of intermediate experiments to guide subsequent experiments in a finite horizon setting. Direct solution of the resulting dynamic programming problem is computationally impractical. Using polynomial chaos surrogates, stochastic optimization methods, and value function approximations, we develop numerical tools to identify sequences of experiments that are optimal for parameter inference, in a computationally feasible manner.

Xun Huan, Youssef M. Marzouk
Massachusetts Institute of Technology
xunhuan@mit.edu, ymarz@mit.edu

MS11
Identification of Polynomial Chaos Representations in High Dimension

The usual identification methods of polynomial chaos expansions in high dimension are based on the use of a series of truncations that induce numerical bias. We first quantify the detrimental influence of this numerical bias, we then propose a new decomposition of the polynomial chaos coefficients to allow performing relevant convergence analysis and identification with respect to an arbitrary measure for the high dimension case.

Guillaume Perrin
Université Paris-Est
Navier (UMR 8205 ENPC-IFSTTAR-CNRS)
pergui85@hotmail.fr

Christian Soize
University of Paris-Est
MSME UMR 8208 CNRS
christian.soize@univ-paris-est.fr

Denis Duhamel
University of Paris-Est
Navier (UMR 8205 ENPC-IFSTTAR-CNRS)
denis.duhamel@enpc.fr

Christine Funfschilling
SNCF
Innovation and Research Department
christine.funfschilling@sncf.fr

MS11
Inverse Problems for Nonlinear Systems via Bayesian Parameter Identification

Inverse problems are important in engineering science and appear very frequently such as for example in estimation of material porosity and properties describing irreversible behaviour, control of high-speed machining processes etc. At present, most of identification procedures have to cope

with ill-possedness as the problems are often considered in a deterministic framework. However, if the parameters are modelled as random variables the process of obtaining more information through experiments in a Bayesian setting becomes well-posed. In this manner the Bayesian information update can be seen as a minimisation of variance. In this work we use the functional approximation of uncertainty and develop a purely deterministic procedure for the updating process. This is then contrasted to a fully Bayesian update based on Markov chain Monte Carlo sampling on a few numerical nonlinear examples. Examples are based on plasticity and nonlinear diffusion models.

Bojana V. Rosic
Institute of Scientific Computing
TU Braunschweig
bojana.rosic@tu-bs.de

Oliver Pajonk
Institute of Scientific Computing
Technische Universität Braunschweig
o.pajonk@tu-bs.de

Alexander Litvinenko
TU Braunschweig, Germany
litvinen@tu-bs.de

Hermann G. Matthies
Institute of Scientific Computing
Technische Universität Braunschweig
wire@tu-bs.de

Anna Kucerova
Faculty of Civil Engineering, Prague, Czech TU
anicka@cml.fsv.cvut.cz

Jan Sykora
Faculty of Civil Engineering
Czech Technical University in Prague
jan.sykora.1@fsv.cvut.cz

MS11
Data Analysis Methods for Inverse Problems

We present exploratory data analysis methods to assess inversion estimates using examples based on l2- and l1-regularization. These methods can be used to reveal the presence of systematic errors s and validate modeling assumptions. The methods include: confidence intervals and bounds for the bias, resampling methods for model validation, and construction of training sets of functions with controlled local regularity.

Luis Tenorio
Colorado School of Mines
ltenorio@mines.edu

MS12
Analysis and Finite Element Approximations of Optimal Control Problems for Stochastic PDEs

In this talk, we consider mathematically and computationally optimal control problems for stochastic partial differential equations. The control objective is to minimize the expectation of a cost functional, and the control is of the deterministic distributed and/or boundary value type. The main analytical tool is the Karhunen-Loeve (K-L) expansion. Mathematically, we prove the existence of an optimal solution and derive optimality system. Computationally, we approximate the optimality system through the discretizations of the probability space and the spatial space by the finite element method; we also derive error estimates in terms of both types of discretizations. Some numerical experiments are given.

Hyung-Chun Lee
Ajou University
Department of Mathematics
hclee@ajou.ac.kr

MS12
Generalized Methodology for Inverse Modeling Constrained by SPDEs

We formulate several stochastic inverse problems to estimate statistical moments (mean value, variance, covariance) or even the whole probability distribution of input data, given the PDF of some response (quantities of physical interest) of a system of SPDEs. The identification objectives minimize the expectation of a tracking cost functional or minimize the difference of desired statistical quantities in the appropriate norms. Numerical examples illustrate the theoretical results and demonstrate the distinctions between the various objectives.

Catalin S. Trenchea
Department of Mathematics
University of Pittsburgh
trenchea@pitt.edu

Max Gunzburger
Florida State University
School for Computational Sciences
mgunzburger@fsu.edu

Clayton G. Webster
Oak Ridge National Laboratory
webstercg@ornl.gov

MS12
Stochastic Inverse Problems via Probabilistic Graphical Model Techniques

We build a graphical model for learning the probabilistic relationship between the input and output of a multiscale problem (e.g. crystal plasticity based deformation). The graphical model is first learned (parameters in potential functions) using a set of training data and suitable optimization strategies (e.g. MLE, EM, etc.). After that, by applying belief propagation algorithm, we can solve the coarse to fine scale inverse problem (e.g. find the initial microstructure given desired properties) or the forward problem (e.g. find the properties resulting from a given initial microstructure).

Nicholas Zabaras, Peng Chen
Cornell University
zabaras@cornell.edu, pc423@cornell.edu

MS12
Least-Squares Estimation of Distributed Random Diffusion Coefficients

We formulate a stochastic inverse problem, estimating the random diffusion coefficient in an elliptic PDE, as a least squares problem in the space of functions with bounded

mixed derivatives. We prove existence and define the necessary optimality conditions using techniques from optimization theory. In addition, the regularization of the problem connects the infinite dimensional problem with its finite noise discretization. Numerical results that validate our theory will be presented.

Hans-Werner van Wyk
Virginia Tech
hvanwyk@vt.edu

Jeff Borggaard
Virginia Tech
Department of Mathematics
jborggaard@vt.edu

MS13
Challenges on Incorporating Uncertainty in Computational Model Predictions

Bayes' theorem allows for the treatment of uncertainties in the whole model prediction process. It can be used for model calibration (either batch or real-time), ranking of scientific hypotheses formulated as mathematical models, ranking of data sets according to information content, and averaging of predictions made by competing models. We discuss the uncertainty quantification research we have been pursuing in the context of realistic models, including sampling with MCMC algorithms and emulation with Gaussian processes.

Ernesto E. Prudencio
Institute for Computational Engineering and Sciences
prudenci@ices.utexas.edu

Gabriel A. Terejanu
Institute for Computational Engineering and Sciences
University of Texas at Austin
terejanu@ices.utexas.edu

MS13
A Stochastic Collocation Approach to Constrained Optimization for Random Data Estimation Problems

We present a scalable, parallel mechanism for identification of statistical moments of input random data, given the probability distribution of some response of a system of stochastic partial differential equations. To characterize data with moderately large amounts of uncertainty, we introduce a stochastic parameter identification algorithm that integrates an adjoint-based deterministic algorithm with the sparse grid stochastic collocation FEM. Rigorously derived error estimates are used to compare the efficiency of the method with other techniques.

Max Gunzburger
Florida State University
School for Computational Sciences
mgunzburger@fsu.edu

Catalin S. Trenchea
Department of Mathematics
University of Pittsburgh
trenchea@pitt.edu

Clayton G. Webster
Oak Ridge National Laboratory
webstercg@ornl.gov

MS13
A Randomized Iterative Proper Orthogonal Decomposition (RI-POD) Technique for Model Identification

In this talk, we shall present a data based technique for the identification of the eigenmodes of very high dimensional linear systems. Our technique is based on the snapshot proper orthogonal decomposition (POD) method. We show that using the snapshot POD with randomized forcing or initial conditions, in an iterative fashion, we can extract as many of the eigenmodes of the linear system as required. The technique works for symmetric as well as non-symmetric systems.

Dan Yu
Texas A&M University
doudouegg@tamu.edu

Suman Chakravorty
Texas A&M University
College Station, TX
schakrav@tamu.edu

MS13
Sparse Bayesian Techniques for Surrogate Creation and Uncertainty Quantification

We develop a multi-output, Bayesian, generalized linear regression model with arbitrary basis functions. The model automatically excludes redundant basis functions while providing access to the full Bayesian predictive distribution of the statistics. By employing a sequentially built tree structure, we are able to demonstrate that it is capable of identifying discontinuities in the response surface. We demonstrate our claims numerically using various basis functions that vary from localized kernels to numerically build Generalized Polynomial Chaos basis.

Nicholas Zabaras
Cornell University
zabaras@cornell.edu

Ilias Bilionis
Center for Applied Mathematics
Cornell University, Ithaca
ib227@cornell.edu

MS14
Application of Goal-Oriented Error Estimation Methods to Statistical Quantities of Interest

The objective here is to present an extension of goal-oriented methods for a posteriori error estimation to the case of stochastic problems with random parameters. We shall consider the stochastic collocation method, for which estimates of statistical moments of the error in a quantity of interest have been proposed in the past, but will focus on estimating the error in these moments themselves and on accurately representing the posterior distribution of the quantity of interest.

Corey Bryant
The University of Texas at Austin
Institute for Computational Engineering and Sciences
cbryant@ices.utexas.edu

Serge Prudhomme
ICES

The University of Texas at Austin
serge@ices.utexas.edu

MS14
Estimating and Bounding Errors in Distributions Propagated via Surrogate Models

We consider the problem of propagating distributions through quantities of interest to differential equations with parameters modeled as random processes. Polynomial chaos expansions approximate random processes, and the differential equations are solved numerically. We estimate discretization error, bound truncation error, and consider the effect of finite sampling in the computed distribution functions for both forward and inverse problems. The results are computable error bounds for distribution functions that we demonstrate with numerical examples.

Troy Butler, Clint Dawson
Institute for Computational Engineering and Sciences
University of Texas at Austin
tbutler@ices.utexas.edu, clint@ices.utexas.edu

Tim Wildey
Sandia National Laboratory
tmwilde@sandia.gov

MS14
An Adjoint Error Estimation Technique Using Finite Volume Methods for Hyperbolic Equations

Many codes exist for hyperbolic equations that employ finite volume methods, which are often nonlinear. A method is presented for adjoint-based *a posteriori* error calculations with finite volume methods. Conditions are derived under which the error in a quantity of interest may be recovered with guaranteed asymptotic accuracy, including for nonlinear forward solvers and weak solutions. We demonstrate the flexibility in implementation of this post-processing technique and accuracy with smooth and discontinuous solutions.

Jeffrey M. Connors
Lawrence Livermore National Laboratory
Center for Applied Scientific Computing
connors4@llnl.gov

Jeffrey W. Banks
Lawrence Livermore National Laboratory
banks20@llnl.gov

Jeffrey A. Hittinger
Center for Applied Scientific Computing
Lawrence Livermore National Laboratory
hittinger1@llnl.gov

Carol S. Woodward
Lawrence Livermore Nat'l Lab
cswoodward@llnl.gov

MS15
Computation of Posterior Distribution in Ordinary Differential Equations with Transport Partial Differential Equations

We consider the estimation of the initial conditions of an Ordinary Differential Equation from a noisy trajectory in a Bayesian setting. The posterior distribution is computed by exploiting the fact that it is transported by the vector field defining the ODE. As a consequence, one can design an iterative computation based on the transport of probability. This transported probability is the solution of a PDE, which is solved by an Eulerian-Lagrangian scheme with bi-orthogonal wavelets.

Nicolas J-B Brunel, Vincent Torri
Universite d'Evry
nicolas.brunel@ensiie.fr, vincent.torri@univ-evry.fr

MS15
Large-scale Seismic Inversion: Elastic-acoustic Coupling, DG Discretization, and Uncertainty Quantification

We present our recent efforts on solving globally large-scale seismic inversion. We begin by a unified framework for elastic-acoustic coupling together with an hp-nonconforming discontinuous Galerkin (DG) spectral element method. Next, consistency, stability, and hp-convergence of the DG method as well as its scalability up to 224k cores are presented. Finally, a method for uncertainty quantification based on the compactness of the data misfit is presented, followed by a brief discussion on a variance-driven adaptivity.

Tan Bui
University of Texas at Austin
tanbui@ices.utexas.edu

Carsten Burstedde
Institut fuer Numerische Simulation
Universitaet Bonn
burstedde@ins.uni-bonn.de

Omar Ghattas, Georg Stadler
University of Texas at Austin
omar@ices.utexas.edu, georgst@ices.utexas.edu

James R. Martin
University of Texas at Austin
Institute for Computational Engineering and Sciences
jmartin@ices.utexas.edu

Lucas Wilcox
University of Texas at Austin
lucasw@ices.utexas.edu

MS15
Nonparametric Estimation of Diffusions: A Differential Equations Approach

We consider estimation of scalar functions that determine the dynamics of diffusion processes. It has been recently shown that nonparametric maximum likelihood estimation is ill-posed in this context. We adopt a probabilistic approach to regularize the problem by the adoption of a prior distribution for the unknown functional. A Gaussian prior measure is chosen in the function space by specifying its precision operator as an appropriate differential operator. We establish that a Bayesian Gaussian conjugate analysis for the drift of one-dimensional non-linear diffusions is feasible using high-frequency data, by expressing the log-likelihood as a quadratic function of the drift, with sufficient statistics given by the local time process and the end points of the observed path. Computationally efficient posterior inference is carried out using a finite element method.

We embed this technology in partially observed situations and adopt a data augmentation approach whereby we iteratively generate missing data paths and draws from the unknown functional. Our methodology is applied to estimate the drift of models used in molecular dynamics and financial econometrics using high and low frequency observations. We discuss extensions to other partially observed schemes and connections to other types of nonparametric inference.

Omiros Papaspiliopoulos
Department of Economics
Universitat Pompeu Fabra
omiros.papaspiliopoulos@upf.edu

Yvo Pokern
Department of Statistical Science, UCL
yvo@stats.ucl.ac.uk

Gareth O. Roberts
Warwick University
gareth.o.roberts@warwick.ac.uk

Andrew M. Stuart
University of Warwick
a.m.stuart@warwick.ac.uk

MS15
A Statistical Approach to Data Assimilation for Hemodynamics

We discuss a Data Assimilation (DA) technique for hemodynamics based on a Bayesian approach. DA is formulated as a control problem minimizing a weighted misfit between data and velocity under the constraint of the Navier-Stokes equations. The control variable is the probability density function of the normal stress at the inflow; we derive statistical estimators (maximum a posteriori and maximum likelihood) and confidence intervals for the velocity. We compare statistical and deterministic estimators.

Alessandro Veneziani
MathCS, Emory University, Atlanta, GA
ale@mathcs.emory.edu

Marta D'Elia
Department of Mathematics and Computer Science
Emory University, Atlanta
mdelia2@emory.edu

MS16
Toward Improving Statistical Components of Multi-scale Simulation Schemes

I will describe an ongoing collaboration with Sorin Mitran and a group of statisticians to develop more sophisticated approaches to handling some issues concerning representation of and communication between kinetic mesoscale PDFs and stochastically simulated microscale data in Mitran's novel time-parallel Continuum-Kinetic-Molecular (tpCKM) method. The mesoscale component of this method can be viewed as an emulator for the microscale dynamics, and our research regards offline and online control of its quality.

Peter R. Kramer
Rensselaer Polytechnic Institute
Department of Mathematical Sciences
kramep@rpi.edu

Sorin Mitran
University of North Carolina Chapel Hill
mitran@unc.edu

Sunli Tang
Rensselaer Polytechnic Institute
Department of Mathematical Sciences
tangs4@rpi.edu

M.J. Bayarri
University of Velacia
susie.bayarri@uv.es

James Berger
Duke University
berger@stat.duke.edu

Murali Haran
Pennsylvania State University
Department of Statistics
mharan@stat.psu.edu

Hans Rudolf Kuensch
ETH Zurich
Department of Mathematics
kuensch@stat.math.ethz.ch

MS16
Improving Gaussian Stochastic Process Emulators

Gaussian Stochastic Process (GASP) emulators are fast surrogates to the output of computationally expensive simulators of complex physical processes used in many scientific applications. They have many advantages, but some improvements are still needed. The talk will present several methods in a Bayesian context for improving the implementation of GASP emulators under computational constraints (including the use of large data sets) and obtaining statistical approximations to the computer model that are closer to the reality.

Danilo Lopes
samsi
danilo@stat.duke.edu

MS16
Emulating Dynamic Models: An Overview of Suggested Approaches

Dynamic models are characterized by a large number of outputs in the time domain and by a strong dependence of outputs conditional on recent past outputs. This makes it difficult to apply standard emulation techniques to such models. Several approaches have been suggested to overcome these problems. The talk will give an overview of these concepts, try to analyze which approach may be most promising under which circumstances, and identify needs for further research.

Peter Reichert
eawag
peter.reichert@eawag.ch

MS16
Statistical Approximation of Computer Model

Output aka Emulation of Simulation

Computer model data can be used to construct a predictor of the computer model output at untried inputs. Such construction combined with assessment of prediction uncertainty is an emulator or surrogate of the computer model. A key strategy uses the Bayes paradigm to produce predictors and quantify uncertainties. An overview of this strategy which uses gaussian stochastic processes as priors will include comments on connections with approaches such as polynomial chaos.

Jerry Sacks
National Institute of Statistical Sciences
sacks@niss.org
sacks@niss.org

MS17
Adaptive Sparse Grids for Stochastic Collocation on Hybrid Architectures

We discuss the algorithmic developments required to build a scalable adaptive sparse grid library tailored for emerging architectures that will allow the solution of very large stochastic problems. We demonstrate the first results of adaptive sparse grids for hybrid systems and detail the algorithmic challenges that were overcome to get these techniques to work on these novel systems.

Rick Archibald
Computational Mathematics Group
Oak Ridge National Labratory
archibaldrk@ornl.gov

MS17
A Compressive Sampling Approach for the Solution of High-dimensional Stochastic PDEs

We discuss a non-intrusive sparse approximation approach for uncertainty propagation in the presence of high-dimensional random inputs. The idea is to exploit the sparsity of the quantities of interest with respect to a suitable basis in order to estimate the dominant expansion coefficients using a number of random samples that is much smaller than the cardinality of the basis.

Alireza Doostan
Department of Aerospace Engineering Sciences
University of Colorado, Boulder
doostan@colorado.edu

MS17
Tensor-based Methods for Uncertainty Propagation: Alternative Definitions and Algorithms

Tensor approximation methods have recently received a growing attention in scientific computing for the solution of high-dimensional problems. These methods are of particular interest in the context of uncertainty quantification with functional approaches, where they are used for the representation of multiparametric functionals. Here, we present different alternatives, based on projection or statistical methods, for the construction of tensor approximations, in various tensor formats, of the solution of parameterized stochastic models.

Anthony Nouy
GeM, L'UNAM Universite, Ecole Centrale Nantes
University of Nantes, CNRS
anthony.nouy@ec-nantes.fr

Billaud Marie
GeM, LUNAM Universite, Ecole Centrale Nantes
Universite de Nantes, CNRS
marie.billaud-friess@ec-nantes.fr

Mathilde Chevreuil
GeM, L'UNAM Universite, Universite de Nantes
Ecole Centrale Nantes, CNRS
mathilde.chevreuil@univ-nantes.fr

Rai Prashant, Zahm Olivier
GeM, L'UNAM Universite, Ecole Centrale Nantes
Universite de Nantes, CNRS
prashant.rai@ec-nantes.fr, olivier.zahm@ec-nantes.fr

MS17
PDE with Random Coefficient as a Problem in Infinite-dimensional Numerical Integration

This talk is concerned with the use of quasi-Monte Carlo methods combined with finite-element methods to handle an elliptic PDE with a random field as a coefficient. A number of groups have considered such problems (under headings such as polynomial chaos, stochastic Galerkin and stochastic collocation) by reformulating them as deterministic problems in a high di- mensional parameter space, where the dimensionality comes from the num- ber of random variables needed to characterise the random field. In recent joint work with Christoph Schwab (ETH) and Frances Kuo (UNSW) we have treated a problem of this kind as one of infinite-dimensional integration - where integration arises because a multi-variable expected value is a multidimensional integral - together with finite-element approximation in the physical space. We use recent developments in the theory and practice of quasi-Monte Carlo integration rules in weighted Hilbert spaces, through which rules with optimal properties can be constructed once the weights are known. The novel feature of this work is that for the first time we are able to design weights for the weighted Hilbert space that achieve what is believed to be the best possible rate of convergence, under conditions on the random field that are exactly the same as in a recent paper by Cohen, DeVore and Schwab on best N-term approximation for the same problem.

Ian H. Sloan
University of New South Wales
School of Mathematics
i.sloan@unsw.edu.au

MS18
A Multiscale Domain Decomposition Method for the Solution of Stochastic Partial Differential Equations with Localized Uncertainties

The presence of numerous localized sources of uncertainties in physical models leads to high dimensional and complex multiscale stochastic models. A numerical strategy is here proposed to propagate the uncertainties through such models. It is based on a multiscale domain decomposition method that exploits the localized side of uncertainties. The separation of scales has the double benefit of improving the conditioning of the problem as well as the convergence of tensor based methods (namely Proper Generalized Decomposition methods) used within the strategy for the separated representation of high dimensional stochastic

parametric solutions.

Mathilde Chevreuil
GeM, L'UNAM Universite, Universite de Nantes
Ecole Centrale Nantes, CNRS
mathilde.chevreuil@univ-nantes.fr

Anthony Nouy
GeM, L'UNAM Universite, Ecole Centrale Nantes
University of Nantes, CNRS
anthony.nouy@ec-nantes.fr

Safatly Elias
LUNAM Universite, Ecole Centrale Nantes, GeM
elias.safatly@ec-nantes.fr

MS18
Greedy Algorithms for Non Symmetric Linear Problems with Uncertainty

Greedy algorithms, also called Progressive Generalized Decomposition algorithms, are known to give very satisfactory results for the approximation of the solution of symmetric uncertain problems with a large number of random parameters. Indeed, their formulation leads to discretized problems whose complexity evolves linearly with respect to the number of parameters, while avoiding the curse of dimensionality. However, naive adaptations of these methods to non-symmetric problems may not converge towards the desired solution. In this talk, different versions of these algorithms will be presented, along with convergence results.

Virginie Ehrlacher
CERMICS - Ecole des Ponts Paristech / INRIA
ehrlachv@cermics.enpc.fr

MS18
Optimized Polynomial Approximations of PDEs with Random Coefficients

We consider the problem of numerically approximating statistical moments of the solution of a partial differential equation (PDE), whose input data (coefficients, forcing terms, boundary conditions, geometry, etc.) are uncertain and described by a finite or countably infinite number of random variables. This situation includes the case of infinite dimensional random fields suitably expanded in e.g Karhunen-Loève or Fourier expansions. We focus on polynomial chaos approximations of the solution with respect to the underlying random variables by either Galerkin projection; Collocation on sparse grids of Gauss points or discrete projection using random evaluations. We discuss in particular the optimal choice of the polynomial space for linear elliptic PDEs with random diffusion coefficient, based on a-priori estimates. Numerical results showing the effectiveness and limitations of the approaches will be presented.

Joakim Beck
Applied Mathematics and Computational Science
KAUST, Saudi Arabia
joba@kth.se

Fabio Nobile
EPFL
fabio.nobile@epfl.ch

Lorenzo Tamellini
MOX, Department of Mathematics
Politecnico di Milano
lorenzo.tamellini@mail.polimi.it

Raul F. Tempone
Mathematics, Computational Sciences & Engineering
King Abdullah University of Science and Technology
raul.tempone@kaust.edu.sa

MS18
Solving Saddle Point Problems with Random Data

Stochastic Galerkin and stochastic collocation methods are becoming increasingly popular for solving (stochastic) PDEs with random data (coefficients, sources, boundary conditions, domains). The former usually require the solution of a large, coupled linear system of equations while the latter require the solution of a large number of small systems which have the dimension of the corresponding deterministic problem. Although many studies on positive definite problems with random data can be found in the literature, there is less work on stochastic saddle point problems, both in terms of approximation theory, and solvers. In this talk, we discuss some of the approximation theory and linear algebra issues involved in applying stochastic Galerkin and collocation schemes to saddle point problems with random data. Model problems that will be used to illustrate the main points, include: 1) a mixed formulation of a second-order elliptic problem (with random diffusion coefficient), 2) the steady-state Navier-Stokes equations (with random viscosity) and 3) a second-order elliptic PDE on a random domain, solved via the fictitious domain method.

Catherine Powell
School of Mathematics
University of Manchester
c.powell@manchester.ac.uk

MS19
Optimization and Model Reduction for Parabolic PDEs with Uncertainties

Optimization of time-dependent PDEs with uncertain coefficients is expensive, because the problem size depends on the spatial and temporal discretization, and on sampling of the uncertainties. I analyze an approach based on stochastic collocation and model reduction, which are used to decouple the subproblems and reduce their sizes. For a class of problems and methods, I prove an estimate for the error between the full and the reduced order optimization problem. Numerical illustrations are provided.

Matthias Heinkenschloss
Department of Computational and Applied Mathematics
Rice University
heinken@rice.edu

MS19
A Stochastic Galerkin Method for Stochastic Control Problems

We examine a physical problem, fluid flow in porous media, which is represented by a stochastic PDE. We first give a priori error estimates for an optimization problem constrained by the physical model. We then use the concept of Galerkin finite element methods to establish a numerical algorithm to give approximations for our stochastic problem. Finally, we develop original computer programs based on the algorithm and present several numerical examples

of various situations.

Jangwoon Lee
University of Mary Washington
llee3@umw.edu

Hyung-Chun Lee
Ajou University
Department of Mathematics
hclee@ajou.ac.kr

MS19
Optimal
Control of Stochastic Flow Using Reduced-order Modeling

We explore an stochastic optimal control problem for incompressible flow by using reduced-order modeling (ROM) based on proper orthogonal decomposition (POD). The POD basis is constructed via a set of "snapshots' obtained by sampling the solution of the Navier-Stokes system at several time instants and over several independent realizations of the random data. Then, the stochastic ROM is constructed via a Galerkin method with respect to the POD basis.

Ju Ming
Florida State University
jming@fsu.edu

Max Gunzburger
Florida State University
School for Computational Sciences
mgunzburger@fsu.edu

MS19
An
Efficient Sparse-Grid-Based Method for Bayesian Uncertainty Analysis

We develop an efficient sparse-grid (SG) Bayesian approach for quantifying parametric and predictive uncertainty of physical systems constrained by stochastic PDEs. An accurate surrogate posterior density is constructed as a function of polynomials using SG interpolation and integration. It improves the simulation efficiency by accelerating the evaluation of the posterior density without losing much accuracy, and by determining an appropriate alternative density which is easily-sampled and captures the main features of the exact posterior density.

Guannan Zhang
Florida State University
gzhang5@fsu.edu

Max Gunzburger
Florida State University
School for Computational Sciences
mgunzburger@fsu.edu

Ming Ye
Department of Scientific computing
Florida State University
mye@fsu.edu

MS20
Fundamental Limitations of Polynomial Chaos Expansions for Uncertainty Quantification in Systems with Intermittent Instabilities

Methods based on truncated Polynomial Chaos Expansion (PCE) have been a popular tool for probabilistic uncertainty quantification in complex nonlinear systems. We show rigorously that truncated PCE have fundamental limitations for UQ in systems with intermittently positive Lyapunov exponents, leading to non-realizability of probability densities and even a blow-up at short times of the second-order statistics. Simple unambiguous examples are used to illustrate these limitations.

Michal Branicki
New York University
branicki@cims.nyu.edu

Andrew Majda
Courant Institute NYU
jonjon@cims.nyu.edu

MS20
Physics-based Auto- and Cross-Covariance Models for Gaussian Process Regression

Gaussian process analysis of systems with multiple outputs is limited by the fact that far fewer good classes of covariance functions exist compared with the single-output case. We propose analytical and numerical auto- and cross-covariance models, which take a form consistent with physical laws governing the underlying simulated process, and are suitable when performing uncertainty quantification or inferences on multidimensional processes (co-kriging). High-order closures are also derived for nonlinear dependencies among the observables.

Emil M. Constantinescu, Mihai Anitescu
Argonne National Laboratory
Mathematics and Computer Science Division
emconsta@mcs.anl.gov, anitescu@mcs.anl.gov

MS20
Covariance Approximation Techniques in Bayesian Non-stationary Gaussian Process Models

Bayesian Gaussian processes have been widely used in spatial statistics but face tremendous computational challenges for very large data sets. The full rank approximation is among the best approximation techniques used recently in statistics to deal with large spatial dataset. This technique is successfully applied in stationary spatial processes where the data are reasonably considered stationary but been tried with real non-stationary large spatial datasets. The goal of this presentation is to generalize this method.

Bledar Konomi, Guang Lin
Pacific Northwest National Laboratory
bledar.konomi@pnnl.gov, guang.lin@pnnl.gov

MS20
Inertial Manifold Dimensionality Finite-time Instabilities in Fluid Flows

We examine the geometry of the inertial manifold associated with fluid flows and relate its nonlinear dimensionality to energy exchanges among different dynamical components. Using dynamical orthogonality we perform efficient order-reduction and we prove and illustrate in 2D Navier-Stokes that the underlying mechanism responsible for the finite dimensionality of the inertial manifold is, apart from

the viscous dissipation, the reverse flow of energy from large to small scales. We discuss implications on data assimilation schemes.

Themistoklis Sapsis
New York University
sapsis@cims.nyu.edu

MS21
A Matrix-Free Approach for Gaussian Process Maximum Likelihood Calculations

In Gaussian processes analysis, the maximum likelihood approach for parameter estimation is limited by the use of the Cholesky factorization on the covariance matrix in computing the likelihood. In this work, we present a stochastic programming reformulation with convergence estimates for solving the maximum likelihood problem for large scale data. We demonstrate that the approach scales linearly with an increase in the data size on a desktop machine, and show some preliminary results on supercomputers with parallel processing.

Jie Chen
Argonne National Lab
jiechen@mcs.anl.gov

MS21
Sequential Optimization of a Computer Model: Whats So Special about Gaussian Processes Anyway?

In computer experiments, statistical models are commonly used as surrogates for slow-running codes. In this talk, the usually ubiquitous Gaussian process models are nowhere to be seen, however. Instead, an adaptive nonparametric regression model (BART) is used to deal with nasty nonstationarities in the response surface. By providing both point estimates and uncertainty bounds for prediction, BART provdes a basis for sequential design criteria to find optima with few function evaluations.

Hugh Chipman
Acadia University, Canada
hugh.chipman@acadiau.ca

Pritam Ranjan
Acadia University
pritam.ranjan@acadiau.ca

MS21
Extracting Key Features of Physical Systems for Emulation and Calibration

Many physical models, such as material strength models, rely on a large number of parameters describe the physical system over a large range of possible input settings. However, for particular model based prediction, the physical complexity of the system is much reduced, and as a result, the effective physical model needed to make predictions may be described by a few functions of the parameters (which we call feature).We present an example where physical understanding and its implementation in the predictive computer code suggest a particular function of material strength to focus on. This allows us to greatly reduce the dimensionality and non-linearity of the problem, making emulation and calibration a much simpler task.

Nicolas Hengartner

Information Sciences Group
Los Alamos National Laboratory
nick@lanl.gov

MS21
Sliced Cross-validation for Surrogate Models

Multi-fold cross-validation is widely used to assess the accuracy of a surrogate model. Despite its popularity, this method is known to have high variability. We propose a method, called sliced cross-validation, to mitigate this drawback. It uses sliced space-filling designs to construct structured cross-validation samples such that the data for each fold are space-filling. Numerical examples and theoretical results will be given to illustrate the proposed method.

Peter Qian
University of Wisconsin - Madison
peterq@stat.wisc.edu

Qiong Zhang
Department of Statistics
University of Wisconsin-Madison
qzhang@stat.wisc.edu

MS22
Simulation Informatics

Modern physical simulations produce large amounts of data. Proper uncertainty quantification on such data sets requires scalable, fault tolerant methods for feature extraction and machine learning. We frame the statistical questions arising from uncertainty quantification as a machine learning problem, which leverages existing work in informatics. We focus particularly on scalable model reduction and surrogate modeling for parameterized simulations – a common scenario in uncertainty quantification.

David F. Gleich
Sandia National Labs
dgleich@purdue.edu

MS22
Scientific Data Mining Techniques for Extracting Information from Simulations

Techniques from scientific data mining have long been used for the analysis of data from various domains including astronomy, remote sensing, materials science, and simulations of turbulence in fluids and plasma. In this talk, I will present some of my work in classification of orbits in Poincare plots in fusion simulations, analysis of coherent structures in Rayleigh-Taylor instability, and comparison of experiments and simulations in Richtmyer-Meshkov instability.

Chandrika Kamath
Lawrence Livermore National Laboratory
kamath2@llnl.gov

MS22
Machine Learning to Recognize Phenomena in Large Scale Simulations

Clustering, classification, and anomaly detection are among the most important problems in machine learning. The existing methods usually treat the individual data

points as the object of consideration. Here we consider a different setting. We assume that each instance corresponds to a group of data points. Our goal is to estimate the distances between these groups and use them to create new clustering and classification algorithms, and recognize phenomena in large scale simulations.

Barnabas Poczos
Carnegie Mellon University
bapoczos@cs.cmu.edu

MS22
Extracting Non-conventional Information in Simulation of Chaotic Dynamical Systems

Many state-of-the-art large scale simulations are chaotic. Examples include turbulent fluid flows using techniques such as direct numerical simulation or large eddy simulation, protein folding using molecular dynamics, and nuclear fusion engineering using plasma dynamics simulation. Performing these simulations often produces very large amounts of data; however, to extract physical insight and understanding from the result of the simulation is nontrivial. This talk focuses on a method of extracting non-conventional information, such as robustness, sensitivity and quantified uncertainty, from the data produced by chaotic simulations. We will discuss methods for identifying the attractor of the chaotic simulation, and introduce the attractor-Fokker-Planck equation that governs the ergodic density on the attractor. We then will introduce our Monte Carlo solver for the adjoint of the Fokker-Planck equation, which can be used to compute the robustness and sensitivity of the chaotic simulation with respect to possible parameter changes. Finally, we will show how the resulting sensitivity can be used for uncertainty quantification.

Qiqi Wang
Massachusetts Institute of Technology
qiqi@mit.edu

MS23
Distinguishing and Integrating Aleatoric and Epistemic Variation in UQ

Much of UQ to date has focused on determining the effect of variables modeled probabilistically, with known distributions. We develop methods to obtain information on a system when the distributions of some variables are known exactly, while others are known only approximately. We use the duality between risk-sensitive integrals and relative entropy to obtain bounds on performance measures over families of distributions. These bounds are computed using polynomial chaos techniques.

Kenny Chowdhary
Brown University
kchowdhary@brown.edu

Jan S. Hesthaven
Brown University
Division of Applied Mathematic
Jan.Hesthaven@Brown.edu

MS23
Stochastic Basis Reduction by QoI Adaptation

We describe a new stochastic model reduction approach that characterizes the uncertainty in predictive models by relying on the dominant subspace occupied by a Quantity of Interest. Orders of magnitude reduction in requisite representation and associated computational costs are achieved in this manner. We demonstrate the methodology on an elliptic problem describing an elastically deforming body.

Roger Ghanem
University of Southern California
Aerospace and Mechanical Engineering and Civil Engineering
ghanem@usc.edu

Ramakrishna Tippireddy
University of Southern California
tipiredd@usc.edu

MS23
Adaptive Basis Selection and Dimensionality Reduction with Bayesian Compressive Sensing

Bayesian inference is implemented to obtain a polynomial chaos expansion for the response of a complex model, given a sparse set of training runs. For polynomial basis reduction, Bayesian compressive sensing is employed to detect basis terms with strong impact on model output via relevance vector machine. Furthermore, a recursive algorithm is proposed to determine the optimal set of basis terms. The methodology is applied to global sensitivity studies of the Community Land Model.

Khachik Sargsyan, Cosmin Safta, Robert D. Berry
Sandia National Laboratories
ksargsy@sandia.gov, csafta@sandia.gov,
rdberry@sandia.gov

Bert J. Debusschere
Energy Transportation Center
Sandia National Laboratories, Livermore CA
bjdebus@sandia.gov

Habib N. Najm
Sandia National Laboratories
Livermore, CA, USA
hnnajm@sandia.gov

Daniel Ricciuto, Peter Thornton
Oak Ridge National Laboratory
ricciutodm@ornl.gov, thorntonpe@ornl.gov

MS23
Stochastic Collocation Methods for Stochastic Differential Equations Driven by White Noise

We propose stochastic collocation methods for time-dependent stochastic differential equations (SDEs) driven by white noise. To control the increasing dimensionality in random space generated by the increments of Brownian motion, we approximate Brownian motion with its spectral expansion. We also use sparse grid techniques to further reduce the computational cost in random space. Numerical examples shows the efficiency of the proposed methods. In particular, our proposed methods can run up to moderately large time with proper schemes in physical space and time.

Zhongqiang Zhang
Brown University

zhongqiang_zhang@brown.edu

George E. Karniadakis
Brown University
Division of Applied Mathematics
george_karniadakis@brown.edu

Boris Rozovsky
Brown University
Boris_Rozovsky@brown.edu

MS24
Probabilistic UQ for PDEs with Random Data: A Case Study

We present a case study for probabilistic uncertainty quantification (UQ) applied to groundwater flow in the context of site assessment for radioactive waste disposal based on data from the Waste Isolation Pilot Plant (WIPP) in Carlsbad, New Mexico. In this context, the primary quantity of interest is the time it takes for a particle of radioactivity to be transported with the groundwater from the repository to man's environment. The mathematical model consists of a stationary diffusion equation for the hydraulic head in which the hydraulic conductivity coefficient is a random field. Once the (stochastic) hydraulic head is computed, contaminant transport can be modelled by particle tracing in the associated velocity field. We compare two approaches: Gaussian process emulators and stochastic collocation combined with geostatistical techniques for determining the parameters of the input random field's probability law. The second approach involves the numerical solution of the PDE with random data as a parametrized deterministic system. The calculation of the statistics of the travel time from the solution of the stochastic model is formulated for each of the methods being studied and the results compared.

Oliver G. Ernst
TU Bergakademie Freiberg
Fakultaet Mathematik und Informatik
ernst@math.tu-freiberg.de

MS24
Proper Generalized Decomposition for Stochastic Navier-Stokes Equations

We propose an application of the Proper Generalized Decomposition to the stochastic Navier-Stokes equations in the incompressible regime. The method aims at determining the dominant components of the stochastic flow by means of suitable reduced bases approximations. The deterministic reduced basis is here constructed using Arnoldi-type iterations, which involve the resolution of a series of deterministic problems whose structure is similar to the original deterministic Navier-Stokes equations such that classical solvers can be re-used. The stochastic solution is then approximated in the reduced space of deterministic modes by means of a Galerkin projection, yielding a low dimensional set of coupled quadratic equations for the stochastic coefficients. The efficiency of the method will be illustrated and its computational complexity will be contrasted with the classical Galerkin Polynomial Chaos method. Computation of the reduced solution residual and of the stochastic pressure field will also be discussed.

Olivier LeMaitre
LIMSI-CNRS
olm@limsi.fr

MS24
Computation of the Second Order Wave Equation with Random Discontinuous Coefficients

In this talk we propose and analyze a stochastic collocation method for solving the second order wave equation with a random wave speed and subjected to deterministic boundary and initial conditions. The speed is piecewise smooth in the physical space and depends on a finite number of random variables. The numerical scheme consists of a finite difference or finite element method in the physical space and a collocation in the zeros of suitable tensor product orthogonal polynomials (Gauss points) in the probability space. This approach leads to the solution of uncoupled deterministic problems as in the Monte Carlo method. We consider both full and sparse tensor product spaces of orthogonal polynomials. We provide a rigorous convergence analysis and demonstrate different types of convergence of the probability error with respect to the number of collocation points for full and sparse tensor product spaces and under some regularity assumptions on the data. In particular, we show that, unlike in elliptic and parabolic problems, the solution to hyperbolic problems is not in general analytic with respect to the random variables. Therefore, the rate of convergence may only be algebraic. An exponential/fast rate of convergence is still possible for some quantities of interest and for the wave solution with particular types of data. We present numerical examples, which confirm the analysis and show that the collocation method is a valid alternative to the more traditional Monte Carlo method for this class of problems. We also present extensions to the elastic wave equation.

Mohammad Motamed
KAUST
mohammad.motamed@kaust.edu.sa

Fabio Nobile
EPFL
fabio.nobile@epfl.ch

Raul F. Tempone
Mathematics, Computational Sciences & Engineering
King Abdullah University of Science and Technology
raul.tempone@kaust.edu.sa

MS24
A Predictor-corrector Method for Fluid Flow Exhibiting Uncertain Periodic Dynamics

Generalized Polynomial Chaos (gPC) is known to exhibit computational difficulties in context of dynamical systems involving random coefficients. This can in particular be attributed to the broadening of the solution spectrum as time evolves. In this work, an iterative numerical method is developed to the computation of almost surely stable limit cycles for the incompressible Navier-Stokes equations subject to random inflow boundary conditions. It relies on the reformulation of the model equations in terms of an uncertain period, which involves a rescaling of the physical time variable. Based on the scaled version, a predictor step estimates the period with respect to a deterministic reference solution. Afterwards, a convex optimization problem is solved to obtain a stochastic correction term to ensure a minimal distance between an initial and terminal state of the trajectory almost surely. An inexact Newton method provides a correction for the initial state such the distance can be decreased even further. The developed numerical method is applied to a benchmark problem given by a flow

around a circular domain subject to uniformly distributed inflow boundary conditions. The numerical results demonstrate the ability of capturing almost surely stable limit cycles with high accuracies, characterized by a vortex shedding scheme with an uncertain period.

Michael Schick
Karlsruhe Institute of Technology
michael.schick@kit.edu

Vincent Heuveline
Institute for Applied and Numerical Mathematics
Karlsruhe Institute of Technology, Universität Karlsruhe
vincent.heuveline@kit.edu

Olivier LeMaitre
LIMSI-CNRS
olm@limsi.fr

MS25

Uncertainty Analysis in the Florida Public Hurricane Loss Model

The Florida Public Hurricane Loss Model was developed for the purpose of predicting annual insured hurricane loss in the state of Florida. The model is an open public model comprised of atmospheric science, engineering, and actuarial science components and it serves as a benchmark against existing proprietary commercial models. This talk will present statistical techniques used to validate the model with a focus on the uncertainty and sensitivity analysis for the loss costs.

Sneh Gulati
Department of Mathematics and Statistics
Florida International University
gulati@fiu.edu

Shahid S. Hamid, Golam Kibria
Florida International University
hamids@fiu.edu, golam.kibria@fiu.edu

Steven Cocke
Center for Ocean-Atmospheric Prediction Studies
The Florida State University
scocke@coaps.fsu.edu

Mark D. Powell
Atlantic Oceanographic and Meteorological Laboratory
National Oceanic and Atmospheric Administration
mark.powell@noaa.gov

Jean-Paul Pinelli
Civil Engineering Department
Florida Institute of Technology
pinelli@fit.edu

Kurtis R. Gurley
Department of Civil and Coastal Engineering
University of Florida
kgurl@ce.ufl.edu

Shu-Ching Chen
School of Computing and Information Sciences
Florida International University
chens@cs.fiu.edu

MS25

Toward Transparency and Refutability in Environmental Modeling

Environmental models would be made more effective by establishing a base set of model fit, sensitivity, and uncertainty measures. Reporting the results of this base set of methods consistently, along with any other methods considered and as innovations in model analysis continue, would improve model transparency and refutability. This work proposes two base set of methods: base set I for all models; base set II for models with shorter execution times

Mary Hill
USGS
mchill@usgs.gov

Dmitri Kavetski
Faculty of Engineering and Built Environment
The University of Newcastle Australia
dmitri.kavetski@newcastle.edu.au

Martyn Clark
National Center for Atmospheric Research
University of Colorado Boulder
mclark@ucar.edu

Ming Ye
Department of Scientific computing
Florida State University
mye@fsu.edu

Mazdak Arabi
Departmet of Civil and Environmental Engineering
Colorado State University
mazdak.arabi@colostate.edu

Laura Foglia
University of California Davis
lfoglia@ucdavis.edu

Steffen Mehl
Department of Civil Engineering
California State University Chico
smehl @ csuchico.edu

MS25

Quantifying and Reducing Uncertainty through Sampling Design

Uncertainty reduction for geo-sphere based projects relies on data collection. A variety of performance measures and associated sample-designs have been proposed. These designs are evaluated on a test problem with a focus on adaptive sampling where information from previous samples is used to identify future sample locations. Example applications of sampling design in from CO_2 sequestration and ground water contaminant detection are presented.

Sean A McKenna
Sandia National Laboratories
samcken@sandia.gov

Jaideep Ray
Sandia National Laboratories, Livermore, CA
jairay@sandia.gov

Bart G. Van Bloemen Waanders

Sandia National Laboratories
bartv@sandia.gov

MS25
Uncertainty Quantification of Shallow Groundwater Impacts due to CO2 Sequestration

A suite of numerical tools including multi-phase and multi-component reactive transport modeling, uncertainty quantification and risk assessment are used to develop risk profiles for the National Risk Assessment Program for CO2 Sequestration. Two quantities, pH and total dissolved solids, were chosen as proxies for assessing shallow groundwater impacts due to CO2 and brine leakage in to the shallow aquifer. A 3D flow and transport model of the Edwards aquifer is used as a site example.

Daniel M. Tartakovsky
University of California, San Diego
dmt@ucsd.edu

Hari Viswanathan
Earth and Environmental Sciences Division
Los Alamos National Laboratory
viswana@lanl.go

Elizabeth Keating, Zhenxue Dai
Los Alamos National Laboratory
ekeating@lanl.gov, daiz@lanl.gov

Rajesh Pawar
Earth and Environmental Sciences Division
Los Alamos National Laboratory
rajesh@lanl.gov

MS26
Random Fluctuations in Homogenization Theory; How Stochasticity Propagates Through Scales

The influence of small scale fluctuations on the solutions of partial differential equations (PDE) is relatively well understood at the most macroscopic level, ie the homogenization level describing the ensemble average of the PDE solution. Many uncertainty quantification contexts require that we understand, at least qualitatively, the random fluctuations of the PDE solution. Much less is known from the theoretical standpoint. This talk will review some existing theories.

Guillaume Bal
Columbia University
Department of Applied Physics and Applied Mathematics
gb2030@columbia.edu

MS26
Uncertainty Quantification in Multi-Scale, Multi-Physics MEMS Performance Prediction

This presentation describes a Bayes network approach to perform comprehensive uncertainty quantification in multi-scale, multi-physics model prediction for a MEMS device. The device performance is related to membrane deflection, affected by multiple physics: creep, damping, contact, and dielectric charging. The Bayes network is able to integrate epistemic and aleatory uncertainty information from multiple sources and activities (modeling, experiments, experts, calibration, verification, validation) and multiple formats (full distributions, sparse data, imprecise data, noise, error estimates).

Sankaran Mahadevan
Vanderbilt University
sankaran.mahadevan@vanderbilt.edu

You Ling
Department of Civil and Environmental Engineering
Vanderbilt University
you.ling@vanderbilt.edu

Joshua Mullins, Shankar Sankararaman
Vanderbilt University
joshua.g.mullins@vanderbilt.edu,
shankar.sankararaman@vanderbilt.edu

MS26
UQ in MD Simulations: Forward Propagation and Parameter Inference

This work focuses on quantifying uncertainty in molecular dynamics (MD) simulations of TIP4P water accounting for intrinsic noise and parametric uncertainty. A functional relationship between selected macroscale observables and uncertain atomistic model parameters is constructed via polynomial chaos expansions using a non-intrusive spectral projection and a Bayesian inference approach. These PC representations are then exploited in an inverse problem involving the estimation of force-field parameters of the TIP4P model using bulk-phase properties of water.

Francesco Rizzi
Department of Mechanical Engineering
Johns Hopkins University
frizzi1@jhu.edu

Omar M. Knio
Duke University
omar.knio@duke.edu

Habib N. Najm
Sandia National Laboratories
Livermore, CA, USA
hnnajm@sandia.gov

Bert J. Debusschere
Energy Transportation Center
Sandia National Laboratories, Livermore CA
bjdebus@sandia.gov

Khachik Sargsyan
Sandia National Laboratories
ksargsy@sandia.gov

Maher Salloum
Sandia National Laboratories
Scalable & Secure Systems Research Department
mnsallo@sandia.gov

Helgi Adalsteinsson
Sandia National Laboratories, Livermore CA
hadalst@sandia.gov

MS26
Quantifying Sampling Noise and Parametric Uncertainty in Coupled Atomistic-Continuum Simu-

lations

We perform a coupled atomistic-to-continuum simulation in a model operating under uncertainty. This latter has the form of parametric uncertainty and sampling noise intrinsic in atomistic simulations. We present mathematical formulations that enable the propagation of uncertainty between the discrete and continuum components and the solution of the exchanged variables in terms of polynomial chaos expansion. We consider a simple Couette flow model where the variable of interest is the wall velocity. Results show convergence of the exchanged variables at a reasonable computational cost.

Maher Salloum
Sandia National Laboratories
Scalable & Secure Systems Research Department
mnsallo@sandia.gov

Khachik Sargsyan
Sandia National Laboratories
ksargsy@sandia.gov

Reese Jones
Co-author
rjones@sandia.gov

Bert J. Debusschere
Energy Transportation Center
Sandia National Laboratories, Livermore CA
bjdebus@sandia.gov

Habib N. Najm
Sandia National Laboratories
Livermore, CA, USA
hnnajm@sandia.gov

Helgi Adalsteinsson
Sandia National Laboratories, Livermore CA
hadalst@sandia.gov

MS27
Evaluation of Mixed Continuous-Discrete Surrogate Approaches

Evaluating the performance of surrogate modeling approaches is essential for determining their viability in uncertainty analysis. To this end, we evaluated categorical regression, ACOSSO splines, Gaussian processes (GPs) with specialized covariance models, and treed GPs on a set of test functions. We describe our evaluation principles and metrics, the characteristics of the test functions considered, and our software testbed. Additionally, we present our numerical results and discuss our observations regarding the merits of each approach.

Patricia D. Hough
Sandia National Laboratories
pdhough@sandia.gov

MS27
Large-scale Surrogate Models

The Bayesian Additive Regression Tree (BART) is a statistical model that represents observed data as a sum of weak learners. Each tree represents a weak learner, and the overall model is a sum of such trees. In this work, we extend the BART model to handle massive datasets using a parellelized MCMC algorithm. Our approach handles datasets too massive to fit on any single data repository, and scales linearly in the number of processor cores.

Matthew Pratola
Los Alamos National Laboratory
mpratola@lanl.gov

MS27
High Performance Bayesian Assessment of Earthquake Source Models for Ground Motion Simulations

Reliable ground motion predictions, with quantified uncertainty, are very important for designing large civil structures. Using Bayesian analysis, we rank candidate kinematic earthquake model classes by comparing their computed quantities of interest (e.g. peak ground velocity, spectral acceleration) against reference attenuation relations. The candidate model classes differ on hypotheses about the physical parameters involved. We report results and give an overview of state of the art parallel statistical algorithms we have been researching.

Ernesto E. Prudencio
Institute for Computational Engineering and Sciences
prudenci@ices.utexas.edu

MS27
Use of Gaussian Process Modeling to Improve the Perez Model in the Study of Surface Irradiance of Buildings

In building energy simulations, a model due to Perez is used to calculate the irradiance received by a tilted surface of a building based on the measurements of the irradiance on a horizontal surface. However, it is known that the prediction from this model can have a substantial discrepancy from the real measurement on a tilted surface. We treat this discrepancy as an integral of an unknown function over the space of the sky dome, and use Gaussian Process to model the integrated values in each small rectangular grid of the sky dome. Nugget is used to stabilize the parameter estimation. Results from different scales of the grid are presented to illustrate this new approach.

Heng Su
Georgia Tech
hsu31@gatech.edu

MS28
Uncertainty Quantification of Building Energy Models

We discuss the NSF funded EFRI-SEED project for risk conscious methods in the design and retrofit of buildings focusing on the quantification of parameter uncertainty in building energy models, at different system scales and different model fidelities. The UQ of the most sensitive parameters is discussed and their influence on building performance predictions is demonstrated. A discussion of how the translation of uncertainties in risk measures will inform design and retrofit decisions concludes the presentation.

Godfried Augenbroe
College of Architecture
Georgia Institute of Technology
godfried.augenbroe@coa.gatech.edu

MS28

An Integrated Approach to Design and Operation of High Performance Buildings in the Presence of Uncertainty

In this talk we introduce how to use uncertainty quantification to leverage the design and operation of high performance buildings. As buildings contain thousands of parameters (from the way they are designed to the way they are occupied and operated), efficient parameter management and identification of critical parameters is the key. We discuss uncertainty and sensitivity analysis in the context of an integrated design process including model calibration, optimization, and failure mode analysis.

Bryan Eisenhower
UCSB
bryane@engr.ucsb.edu

MS28

UQ for Better Commercial Buildings: From Design to Operation

Commercial buildings are expensive assets characterized by long lives and significant environmental and economic impact; demanding great care in both their design as well as ongoing operation. This talk discusses UQ for the robust design of high-performance buildings, their improved operation using model based predictive control that relies on reduced order models and extracted near optimal rule sets in the face of uncertainty in human behavior, and fault detection and diagnosis for existing buildings.

Gregor Henze
University of Colorado at Boulder
gregor.henze@Colorado.EDU

MS28

Sensitivity of Building Parameters with Building Type, Climate, and Efficiency Level

As one embarks on building an energy model of an existing building there are parameters that are known, somewhat unknown, and very unknown. Based on the type of building, the climate it is operating in, and its energy use intensity, the uncertainty of the simulations energy results based on the results sensitivity to the known and unknown parameters variations. Results will be presented of several hundred thousand simulations showing these uncertainties and their corresponding parameter sensitivities.

John Kennedy
Autodesk
john.kennedy@autodesk.com

MS28

Uncertainty Quantification Methods for Multiphysics Applications

Uncertainty quantification is increasingly recognized as a key component in modeling and simulation-based science and engineering. There are, however, many UQ challenges for large-scale applications including expensive model evaluation, large parameter space with complex correlations, highly nonlinear models, diverse data sources for calibration, model-form uncertainties, etc. This talk surveys current techniques for these challenges and also describes a LLNL software package called PSUADE that captures many such techniques, may be applicable to energy efficiency applications.

Charles Tong
Lawrence Livermore National Laboratory
chtong@llnl.gov

MS29

Application of the Implicit Particle Filter to a Model of Nearshore Circulation

Data assimilation is properly viewed as an exercise in conditional probabilities. Models of the ocean and atmosphere have typical state dimensions of $O(10^5 - 10^7)$, so direct calculation of the relevant pdfs is not practical and we must apply Monte-Carlo methods. We present results from an efficient Monte-Carlo method in which the conditional pdf is sampled directly. We show applications of the method to high dimensional systems.

Robert Miller
College of Oceanic and Atmospheric Sciences
Oregon State University, Corvallis
miller@coas.oregonstate.edu

MS29

Implicit Particle Filtering for Geomagnetic Data Assimilation

A large amount of data of the earths magnetic field has recently become available due to satellite missions. This data can be used to improve the predictions of geomagnetic models and the interest in data assimilation techniques has thus grown in this field. Thus far, a 4D-Var approach and a Kalman filter have been considered. Here, the implicit particle filter is applied and its performance is compared to two competing Monte Carlo algorithms.

Matthias Morzfeld
Department of Mathematic
Lawrence Berkeley National Laboratory
mmo@math.lbl.gov

MS29

A Tutorial on Implicit Particle Filtering for Data Assimilation

I will give an introduction to implicit sampling, a new methodology that finds high-probability samples of multi-dimensional probability densities by solving equations with a random input. The implicit sampling strategy focuses attention on regions of high probability and, thus, is applicable even if the state dimension is large. I will present details of implicit sampling in connection with data assimilation and will provide several examples to illustrate the efficiency and accuracy of the algorithm.

Xuemin Tu
University of Kansas
Lawrence, KS 66045-7594
xtu@math.ku.edu

MS29

An Application of Rare Event Tools to a Bimodal Ocean Current Model

I will review some recent results on importance sampling methods for rare event simulation as well as discuss their application to the filtering problem for a simple model of

the Kuroshio current. Assuming a setting in which both observation noise and stochastic forcing are present but small, I will demonstrate numerically and theoretically that sophisticated importance sampling techniques can achieve very small statistical error. Standard filtering methods deteriorate in this small noise setting.

Jonathan Weare
University of Chicago
Department of Mathematics
weare@math.uchicago.edu

Eric Vanden-Eijnden
Courant Institute
New York University
eve2@cims.nyu.edu

MS31

Multiple Computer Experiments: Design and Modeling

A growing trend in uncertainty quantification is to use multiple computer experiments to study the same complex system. We construct a new type of design, called a sliced orthogonal array based Latin hypercube design, intended for efficiently running such experiments. Such a design itself achieves attractive uniformity and can be sliced into Latin hypercube designs. This sliced structure also leads to a two-stage modeling strategy for integrating data from multiple computer experiments.

Youngdeok Hwang, Xu He
Department of Statistics
University of Wisconsin-Madison
hwang@stat.wisc.edu, hexu@stat.wisc.edu

Peter Qian
University of Wisconsin - Madison
peterq@stat.wisc.edu

MS31

Efficient Analysis of High Dimensional Data in Tensor Formats

In this article we introduce new methods for the analysis of high dimensional data in tensor formats, where the underling data come from the stochastic elliptic boundary value problem. We approximate the high dimensional operator via sums of elementary tensors. This tensors representation can be effectively used for computing different values of interest, such as maximum norm, level sets and cumulative distribution function. As an intermediate step we describe efficient iterative algorithms for computing the characteristic and sign functions as well as pointwise inverse in the canonical tensor format.

Alexander Litvinenko
TU Braunschweig, Germany
litvinen@tu-bs.de

MS31

An Adaptive Sparse Grid Generalized Stochastic Collocation Method for High-dimensional Stochastic Simulations

Our modern treatment of predicting the behavior of physical and engineering problems relies on approximating solutions in terms of high dimensional spaces, particularly in the case when the input data (coefficients, forcing terms, boundary conditions, geometry, etc) are affected by large amounts of uncertainty. To approximate these higher dimensional problems we present an adaptive sparse grid generalized stochastic collocation technique constructed from both global polynomial approximations and local multiresolution decompositions. Rigorously derived error estimates, for the fully discrete problem, will be used to show the efficiency of the methods at predicting the behavior of both smooth and/or discontinuous solutions.

Clayton G. Webster
Oak Ridge National Laboratory
webstercg@ornl.gov

Max Gunzburger
Florida State University
School for Computational Sciences
mgunzburger@fsu.edu

Fabio Nobile
EPFL
fabio.nobile@epfl.ch

Raul F. Tempone
Mathematics, Computational Sciences & Engineering
King Abdullah University of Science and Technology
raul.tempone@kaust.edu.sa

MS31

Uncertainty Quantification for Overcomplete Basis Representation in Computer Experiments

Overcomplete basis representation is a surrogate model formed by a linear combination of overcomplete basis functions. The method can be effectively used to mimic complicated and non-stationary response surfaces in computer experiments or numerical approximation. The coefficients in the model are inferred via the matching pursuit technique based on a sparse model assumption. Prediction is made based on the fitted model. Because it is a numerical method without a stochastic structure, it cannot readily give an assessment of the prediction uncertainty. We use a Bayesian approach to impose a multivariate normal prior on the collection of the coefficients in the overcomplete basis representation. Since this is a large dictionary, the prior is over a very large space. But the number of significant coefficients in the representation is usually much smaller (called effect sparsity in design of experiments). For a given data, we can thus collapse the large space to a manageable size. This collapsing is achieved by using a Bayesian variable selection technique called stochastic search variable selection. Once the Bayesian framework is formulated, UQ can be readily implemented but the computational details need to be worked out. The proposed UQ approach can be used to simulate posterior samples for the predicted model, from which Bayesian credible intervals are constructed. Numerical study in two cases demonstrates the success of the approach. (Based on joint work with R. B. Chen, W. C. Wang, and Rui Tuo.)

Jeff Wu
Georgia Institute of Technology
jeffwu@isye.gatech.edu

MS32

Computational Nonlinear Stochastic Homogenization Using a Non-concurrent multiscale Approach

for Hyperelastic Heterogeneous Microstructures Analysis

We present an analysis of the effects of stochastic dimension on a solver based on a tensorial product decomposition for studying propagation of uncertainties in nonlinear boundary value problems. An application to computational nonlinear stochastic homogenization for hyperelastic heterogeneous materials, where the geometry of the microstructure is random, is proposed.

Alexandre Clément
Université Paris-Est, Laboratoire Modélisation et Simulation
Multi Echelle, MSME UMR 8208 CNRS
alexandre.clement@univ-mlv.fr

Christian Soize
University of Paris-Est
MSME UMR 8208 CNRS
christian.soize@univ-paris-est.fr

MS32
Pink and $1/f^\alpha$ Noise Inputs in Stochastic PDEs

We consider colored noise having a power spectrum that decays as $1/f^\alpha$, where f denotes the frequency and $\alpha \in (0, 2]$. We study, in the context of both 1-D and 2-D differential equations, methods for modeling random inputs as $1/f^\alpha$ random fields. We show that the solutions to differential equations exhibit a strong dependence on α, indicating that further examination of how randomness in differential equation is modeled and simulated is warranted.

John Burkardt
Department of Computational Science
Florida State University
jburkardt@fsu.edu

Max Gunzburger
Florida State University
School for Computational Sciences
mgunzburger@fsu.edu

Miroslav Stoyanov
Florida State University
Department of Scientific Computing
mkstoyanov@gmail.com

MS32
Efficient Algorithm for Computing Rare Failure Probability

Evaluation of failure probability is a fundamental task in many important applications such as aircraft design, risk management, etc. Mathematically it can be formulated easily as integrals. The difficulty lies in the fact that the integrals are usually of high dimensions and more importantly the geometry is irregular and known only through simulations of some complex systems under consideration. In practical applications when full-scale simulations are time consuming, there exists no effective methods to accurately compute failure probability. The situation is more severe when dealing with rare failure probability, i.e, failure probability less than 10^{-5}. In this work we discuss the strength and limitation of the existing popular methods. We further present an efficient algorithm to simulate failure probability accurately at very low simulation cost. The algorithm is able to capture rare failure probability

with only a few hundreds simulations and is suitable for practical complex system. Both mathematical analysis and numerical examples are provided.

Jing Li, Dongbin Xiu
Purdue University
li176@purdue.edu, dxiu@purdue.edu

MS32
Hierarchical Multi-output Gaussian Process Regression for Uncertainty Quantification with Arbitrary Input Probability Distributions

We develop an efficient, fully Bayesian, non-intrusive framework for uncertainty quantification of computer codes. A hierarchical treed Gaussian process surrogate is built by adaptively decomposing the stochastic space in a sequential manner that calls upon Bayesian Experimental Design techniques for data gathering. The resulting surrogate provides point estimates as well as error-bars for the statistics of interest. We demonstrate numerically that the suggested framework can resolve local, non-isotropic features, e.g., discontinuities, slowly varying dimensions, etc.

Ilias Bilionis
Center for Applied Mathematics
Cornell University, Ithaca
ib227@cornell.edu

Nicholas Zabaras
Cornell University
zabaras@cornell.edu

MS33
Uncertainty in Geotechnical Engineering

The lecture will focus on the applications of probabilistic techniques to different problems in Geotechnical engineering. The theoretical background, including representation of uncertainty on soil properties by means of random fields will be briefly presented. A number of examples will illustrate the important contribution of probabilistic techniques to the assessment of geotechnical structures safety and reliability and to decision taking in Geotechnical Engineering, including earth and rockfill dams, foundations, tunnels and shafts.

Gabriel Auvinet-Guichard
Instituto de Ingenieria
Universidad Nacional Autonoma de Mexico, UNAM
gauvinetg@iingen.unam.mx

MS33
Causality and Stochastic Processes with Varying Evidence Conditions

A methodology for introducing Causality and Stochastic Processes into the probabilistic solution of inverse problems is presented. This is based on the representation on causal events by the use of Bayesian Networks when coupled to different schemes of evidence availability. Particularly when evidence varies (data, model predictions and even expert's beliefs) and this can be represented as stochastic processes. Illustrative cases including Multi-Physics Geomechanics, Natural Hazards and Energy-Based Developments are discussed.

Zenon Medina-Cetina

Zachry Department of Civil Engineering
Texas A&M University
zenon@tamu.edu

MS33
Modelling Uncertainty in Risk Assessment for Natural Hazards

Optimal strategies for natural hazards risk mitigation, risk analysis professionals must assess and quantify hazard, vulnerability and risk in the context of safety. These are subject to major uncertainties. Uncertainty in different steps of the analysis is often categorized into alreatory (natural variability) and epistemic (due to lack of knowledge). Examples that illustrate how the uncertainty is modeled in quantitative risk analysis, and the shortcomings of the existing methods, will be presented.

Farrokh Nadim
International Centre for Geohazards ICG
Norwegian Geotechnical Institute NGI
farrokh.nadim@ngi.no

MS33
Estimation of Multiscale Fields Representing Anthropogenic CO2 Emissions from Sparse Observations

We investigate spatial models of anthropogenic CO2 emissions for use in inverse problems. Socioeconomic methods of CO2 emissions estimation show that their spatial distribution is strongly multiscale. We investigate the use of easily observed proxies e.g., images of nightlights and population density for emission modeling. We consider bases drawn from them e.g. bivariate Gaussian kernels, or combine them to develop reduced wavelet representations. We perform trade-offs between model complexity, reconstruction accuracy and the uncertainty.

Jaideep Ray
Sandia National Laboratories, Livermore, CA
jairay@sandia.gov

Bart G. Van Bloemen Waanders, Sean A McKenna
Sandia National Laboratories
bartv@sandia.gov, samcken@sandia.gov

MS34
Challenges in Devising Manufactured Solutions for PDE Applications

We describe some challenges we've encountered in devising manufactured solutions to specific PDE applications and the ways in which the challenges were met. The applications are Darcy flow with discontinuous permeability coefficient, free surface flow with kinematic boundary condition, the solute transport equations, and the drift-diffusion equations. The examples demonstrate the flexibility and wide applicability of manufactured solutions, along with some limitations.

Patrick M. Knupp
Sandia National Laboratories
pknupp@sandia.gov

MS34
The Requirements and Challenges for Code Verification Needed to Support the Use of Computational Fluid Dynamics for Nuclear Reactor Design and Safety Applications

Today, computational fluid dynamics (CFD) is being used extensively in support of nuclear reactor design and safety analysis. Verification and Validation (VV) are the technical tools (processes) by which CFD simulation credibility is quantified. In particular, code verification, solution verification, and validation are coupled into an overall process for assessing the accuracy of the computed CFD solution. This presentation will discuss some of the specific requirements, as well as challenges, for code verification needed to support of the use of CFD for nuclear reactor design and safety applications.

Hyung B. Lee
Bettis Laboratory
leehb@bettis.gov

MS34
Tools and Techniques for Code Verification using Manufactured Solutions

Verifying computational science software using manufactured solutions requires the generation of the solutions with associated forcing terms and their reliable implementation in software. There are several issues that arise in generating solutions, including ensuring that they are meaningful, and the algebraic complexity of the forcing terms. Addressing these issues within the open source Manufactured Analytical Solution Abstraction (MASA) library, which is designed to provide a reliable platform for verification with manufactured solutions, will be discussed.

Nicholas Malaya, Roy Stogner, Robert D. Moser
University of Texas at Austin
nick@ices.utexas.edu,   roystgnr@ices.utexas.edu,
rmoser@ices.utexas.edu

MS34
Code Verification: Practices and Perils

As scientific codes become more complex through use of sophisticated algorithms, parallelization procedures and layers of interfaces, probability for implementation mistakes that affect the computed solution increases. In this environment, rigorous code verification through use of order-of-accuracy studies becomes essential to provide confidence that the intended code solves its governing equations correctly. We will discuss a set of best practices for code verification and some common issues that arise in their use.

Carol S. Woodward
Lawrence Livermore Nat'l Lab
cswoodward@llnl.gov

MS35
Practical UQ for Engineering Applications with DAKOTA

Through DAKOTA, we strive to deploy general-purpose UQ software to a broad range of engineering applications, supporting risk-informed design. Practical engineering UQ methods must manage simulation cost, nonlinearity, non-smoothness, and potentially large parameter spaces. Emerging reliability, stochastic expansion, and interval estimation algorithms in DAKOTA address these challenges. These can be employed in mixed determinis-

tic/probabilistic analyses such as optimization under uncertainty. This talk will highlight application and environment complexities that can limit efficient uncertainty quantification.

Brian M. Adams
Sandia National Laboratories
Optimization/Uncertainty Quantification
briadam@sandia.gov

Laura Swiler
Sandia National Laboratories
Albuquerque, New Mexico 87185
lpswile@sandia.gov

Michael S. Eldred
Sandia National Laboratories
Optimization and Uncertainty Quantification Dept.
mseldre@sandia.gov

MS35
Exact Calculations for Random Variables in Uncertainty Quantification Using a Computer Algebra System

The Maple-based APPL language performs exact probability calculations involving random variables. This talk introduces the langauge and presents several applications, including bootstrapping, goodness-of-fit, reliability, probability distribution selection, stochastic activity networks, time series analysis, and transient queueing analysis.

Lawrence Leemis
College of William and Mary
leemis@math.wm.edu

MS35
Open TURNS: Open source Treatment of Uncertainty, Risk 'N Statistics

The needs to assess robust performances for complex systems have lead to the emergence of a new industrial simulation challenge: to take into account uncertainties when dealing with complex numerical simulation frameworks. Open TURNS is an Open Source software platform dedicated to uncertainty propagation by probabilistic methods, jointly developed since 2005 by EDF RD, EADS Innovation Works, and PhiMECA. This talk gives an overview of the main features of the software from a user's viewpoint.

Anne-Laure Popelin
EDF R&D
anne-laure.popelin@edf.fr

Anne Dutfoy
EDF, Clamart, France
Anne.Dutfoy@edf.fr

Paul Lematre
EDF R&D
INRIA Bordeaux
paul.lemaitre@edf.fr

MS35
HPD Liberates Applied Probability AND Enables Comprehensively Tackling Design Engineering

HPD, which stands for *Holistic Probabilistic Design*, consists of a *methodology* and two breakthrough *software suites* for probabilistically tackling problems of any complexity in Design Engineering. Initially developed at Xerox Corporation where variability of thousands of characteristics affecting system performance dominated product development efforts, the HPD software, in fact, *liberates Applied Probability* and has *exposed shortfalls* of existing techniques! As importantly, *HPD revolutionizes Stochastic Analysis and Optimization* for manufacturing industries!

Jean Parks, Chun Li
Variability Associates
jparks20@cox.net, chiminli598@yahoo.com

MS36
Local-Low Dimensionality of Complex Atmospheric Flows

We are investigating complex atmospheric flows in Owens Valley, California, using the Weather Research and Forecasting (WRF) Model. Owens Valley is particularly interesting since it displays complex flows, including clear-air turbulence and atmospheric rotors. We are exploring whether a Local Ensemble Transform Kalman Filter (LETKF) data assimilation scheme works well in such a geographical setting. This work determines how small of an effective dimension the atmospheric dynamics reduce to over such a terrain.

Thomas Bellsky
Michigan State University
Department of Mathematics
bellskyt@asu.edu

MS36
Assimilation of Thermodynamic Profiler Retrievals in the Boundary Layer: Comparison of Methods and Observational Error Specifications

A 2009 National Research Council report recommended investing in a nationwide network of thermodynamic profiling instruments for the atmospheric boundary layer to better forecast mesoscale storm and rainfall events. In this work, we complement the efforts of *Otkin et al* (2011) and *Hartung et al* (2011) by considering variational and hybrid data assimilation frameworks, and different approximations of the retrieved observation error covariance matrices.

Sean Crowell
National Severe Storms Laboratory
Norman, OK
sean.crowell@noaa.gov

Dave Turner
National Severe Storms Laboratory
NOAA
dave.turner@noaa.gov

MS36
Lagrangian Data Assimilation and Control: Hide and Seek

Data Assimilation is the act of merging observed quantities of a physical system into a Mathematical model to provide an estimate of the state. The Lagrangian framework is utilised when the observations are of positions of underwater autonomous vehicles that move with the flow

field. In this talk I will incorporate the Data Assimilation framework with techniques developed in control theory to provide a novel approach in inferring on important structures of the flow field.

Damon Mcdougall
University of Warwick
United Kingdom
d.mcdougall@warwick.ac.uk

MS36
Uncertainty Quantification and Data Assimilation in Multiscale Systems Using Stochastic Homogenization

We study ensemble Kalman filtering on a low-dimensional multiscale system with fast and slow metastable regimes. We find that, surprisingly, a reduced forecast model with stochastic parametrization of the fast dynamics can better capture transitions between slow metastable states than when using the higher-dimensional, perfect deterministic model. This is explained in terms of greater reliability of the ensemble or improved ensemble spread using the stochastic model. Implications for stochastic parametrizations in data assimilation are discussed.

Lewis Mitchell
The University of Sydney
Lewis.Mitchell@uvm.edu

Georg A. Gottwald
School of Mathematics and Statistics
University of Sydney
gottwald@maths.usyd.edu.au

MS37
Overview of Volcanic Hazard Assessment

Straight Monte-Carlo determination of the probability of rare catastrophic volcanic events is not possible. Our strategy uses a GaSP emulator to determine the region of the input space defining the catastrophic event. A suitable distribution on the inputs is then used to determine the probability of this region. Adequate handling of the many uncertainties present is possible by quantifying all uncertainties in terms of probability distributions and combining them in a Bayesian analysis.

M.J. Bayarri
University of Velacia
susie.bayarri@uv.es

MS37
Modeling Large Scale Geophysical Flows: Physics and Uncertainty

Mathematical simulations of volcanic mass flows supplement field deposit studies, providing data from which to make predictions of volcanic hazards. Several parameters and functions must be specified upon input, in order to start the simulation. These inputs include the total volume of the mass flow, the initial direction of the flow, friction and dissipation factors, and the terrain over which the mass moves. These inputs are often poorly characterized, or are known to be inaccurate, and these inaccuracies affect the simulation outputs. Here we study the interplay between the physics of geophysical flows and the uncertain inputs, and examine the effect of uncertainty on outputs, in order

to provide a quantitative measure of hazard at locations downstream from the volcano. This approach draws on insight from the geo-science community, methods of high performance computing, and novel use of Bayesian statistics and mathematical modeling.

E. Bruce Pitman
Dept. of Mathematics
Univ at Buffalo
pitman@buffalo.edu

M.J. Bayarri
University of Velacia
susie.bayarri@uv.es

James Berger
Duke University
berger@stat.duke.edu

Eliza Calder
University of Buffalo
ecalder@buffalo.edu

Abani K. Patra
SUNY at Buffalo
Dept of Mechanical Engineering
abani@eng.buffalo.edu

Elaine Spiller
Marquette University
elaine.spiller@marquette.edu

Robert Wolpert
Duke University
wolpert@stat.duke.edu

MS37
Design and Use of Surrogates in Hazard Assessment

It is the rare, but large volume events that will cause some location of interest to be inundated by a volcanic flow. Standard statistical sampling techniques would focus too many samples (e.g. volcanic flow simulations) on small volume events. Using a statistical emulator of flow simulations, we can focus attention on these infrequent but high-consequence events and construct a boundary in parameter space at the smallest volume events that would inundate a location of concern.

Elaine Spiller
Marquette University
elaine.spiller@marquette.edu

MS37
Combining Deterministic and Stochastic Models For Hazard Assessment

The deterministic flow model "TITAN-2D" predicts course, depth, and velocity for pyroclastic flows following a dome collapse events of specified volumes and initial directions, for a region whose topography is available as digital elevation maps (DEMs). I describe how to combine evidence from TITAN-2D, a rapid stochastic emulator, and heavy-tailed stochastic models of flow volumes and directions, to quantify the hazard of a catastrophic inundation at specified locations, reflecting uncertainty about the models and

data.

Robert Wolpert
Duke University
wolpert@stat.duke.edu

Elaine Spiller
Marquette University
elaine.spiller@marquette.edu

MS38
Numerical Strategies for Epistemic Uncertainty Analysis

Most of the existing UQ analysis tools rely on the knowledge of the probability distribution of the uncertain inputs, also known as aleatory uncertainty. In practice, more often one does not possess sufficient amount of knowledge to completely specify the distributions of the input uncertainty — epistemic uncertainty. And most of the existing tools of UQ do not readily apply. In this talk we discuss some numerical strategies to efficiently quantify the impacts of epistemic uncertainty. The methods are based on numerically creating accurate surrogate of the problem, without the need of input probability distributions. And probabilistic analysis can then be conduct in a post-processing step, without incurring additional simulation effort. We present the numerical algorithms, their convergence analysis, and examples to demonstrate the effectiveness of the strategies.

Xiaoxiao Chen
Purdue University
chen294@math.purdue.edu

Eun-Jae Park
Dept of Computational Science and Engineering-WCU
Yonsei University
ejpark@yonsei.ac.kr

Dongbin Xiu
Purdue University
dxiu@purdue.edu

MS38
A Localized Strategy for Generalized Polynomial Chaos Methods

We present a numerical strategy to treat stochastic differential equations in high dimensions. The approach utilizes a local generalized polynomial chaos (gPC) expansion to approximate the solution in "elements". And such a local expansion can be low dimensional. Then connecting conditions are imposed to enforce the solution to satisfy the desired mathematical properties of the original differential equations. When properly implemented, the method can reduce a high-dimensional SPDE in the global domain into a group of much lower dimensional SPDEs in elements. And the simulation speed-up could be highly significant. We will discuss the technical details of the approach and use examples to demonstrate its efficiency.

Yi Chen, Dongbin Xiu
Purdue University
chen411@purdue.edu, dxiu@purdue.edu

MS38
Stochastic Integration Methods and their Application to Reliability Analysis

Among the most popular methods for computing failure probabilities is FORM. If the curvature of the failure function is large, FORM is known to become inaccurate. Under certain conditions the failure integral may be carried over to an expectation value. The computation of this integrals leads to high dimensional integration over the random space. Several sparse grid integration methods are considered and compared on test examples from literature. The complete method is applied to the life cycle of a wheel set of a train.

Utz Wever
Siemens AG
utz.wever@siemens.com

Albert B. Gilg
Siemens AG
Corporate Technology
albert.gilg@siemens.com

Meinhard Paffra
Siemens AG
meinhard.paffrath@siemens.com

MS38
Uncertainty Quantification with High Dimensional, Experimentally Measured Inputs

In this work, we tackle in a holistic manner the problem of uncertainty quantification in the presence of high-dimensional, experimentally measured inputs. Non-linear model reduction techniques are used to reduce the dimensionality of the experimentally observed input and estimate its probability density. A surrogate of the underlying system is created via interplay of High Dimensional Model Reduction (HDMR/ANOVA) and the treed Bayesian regression frameworks developed recently by our group. Numerical emphasis is given in uncertainty quantification of flow through porous media.

Ilias Bilionis
Center for Applied Mathematics
Cornell University, Ithaca
ib227@cornell.edu

Nicholas Zabaras
Cornell University
zabaras@cornell.edu

MS39
Several Interesting Parabolic Test Problems

An important consideration for a posteriori error estimation methods is their performance on nonlinear PDEs for problems that involve weak solution features or other degeneracies. Typically, the errors in such regions are large, and nonlinear aspects of the error evolution cannot be neglected. To test error estimation techniques in this regime, we have formulated several problems based on nonlinear, parabolic PDEs. We will discuss these problems and demonstrate results from the nonlinear error transport method.

Jeffrey A. Hittinger
Center for Applied Scientific Computing
Lawrence Livermore National Laboratory
hittinger1@llnl.gov

Jeffrey W. Banks
Lawrence Livermore National Laboratory
banks20@llnl.gov

Jeffrey M. Connors
Lawrence Livermore National Laboratory
Center for Applied Scientific Computing
connors4@llnl.gov

Carol S. Woodward
Lawrence Livermore Nat'l Lab
cswoodward@llnl.gov

MS39
Exact Error Behavior of Simple Numerical Problems

Although there is significant mathematical literature regarding convergence analysis, actual testing of codes is done by numerical experiment. The gap between numerical results and mathematical theory leaves many questions unanswered. The most important being, how do we know the observed convergence rate is the asymptotic one? In this paper we outline a class of exact solutions for the modified equation that allow us to explore this and other questions in a more rigorous manner.

Daniel Israel
Los Alamos National Laboratory
dmi1@lanl.gov

MS39
Verification and Validation in Solid Mechanics

Verification and validation in solid mechanics lags behind other disciplines, possibly because of the larger number of variables involved. Verification in solid mechanics must extend from small deformations using simple constitutive models to large deformations using complicated constitutive models. Innovative large-deformation manufactured solutions, applicable to history-dependent materials, are presented. Also, novel visualizations of stress states actually reached in applications are used to expose the need for experiments involving transient loading under massive deformations.

Krishna Kamojjala, Rebecca Brannon
University of Utah
krishna.kamojjala@gmail.com, rebecca.brannon@utah.edu

MS39
Cross-Application of Uncertainty Quantification and Code Verification Techniques

In most applications, sensitivity analysis (SA) and uncertainty quantification (UQ) ignore numerical error when applied to data from computer simulations, but in this work, numerical error is the focus. The differences in SA results for models with and without numerical error are examined, with implications for SA and UQ consumers. Then, UQ techniques are used to directly investigate the truncation error of numerical methods.

V. Gregory Weirs
Sandia National Laboratories
vgweirs@sandia.gov

MS40
Sampling and Inference for Large-scale Inverse Problems Using an Optimization-based Approach

In the Bayesian approach to inverse problems, a posterior probability density function is written down that depends upon the likelihood and prior probability density functions. Estimators for unknown parameters can then be computed, and uncertainty quantification performed, using output from an MCMC method which samples from the posterior. In this talk, the focus is on efficient MCMC sampling techniques for large-scale inverse problems that make using of optimization algorithms.

Johnathan M. Bardsley
University of Montana
bardsleyj@mso.umt.edu

MS40
Approximate Marginalization of Uninteresting Distributed Parameters in Inverse Problems

In the Bayesian inversion framework, all unknowns are treated as random variables and all uncertainties can be modeled systematically. Recently, the approximation error approach was proposed for handling model errors due to unknown nuisance parameters and model reduction. In this approach, approximate marginalization of these errors is carried out before the estimation of the interesting variables. We discuss the adaptation of the approximation error approach for approximate marginalization of uninteresting distributed parameters in inverse problems.

Ville P. Kolehmainen
Department of Applied Physics
University of Eastern Finland
ville.kolehmainen@uef.fi

Jari P Kaipio
Department of Applied Physics, University of Eastern Finland
2Department of Mathematics, University of Auckland
jari@math.auckland.ac.nz

Tanja Tarvainen
Department of Applied Physics
University of Eastern Finland
tanja.tarvainen@uef.fi

Simon Arridge
University College London
S.Arridge@cs.ucl.ac.uk

MS40
Recovery from Modeling Errors in Non-stationary Inverse Problems: Application to Process Tomography

In non-stationary inversion, time-varying targets are estimated based on measurements collected during the evolutions of the targets. In the reconstructions, evolution models of the targets are utilized. The solutions of inverse problems are sensitive to errors in the models. We demonstrate that in some cases, however, it is possible to recover from modeling errors by statistical modeling of the error sources. As an example case, we consider imaging of moving fluids in industrial process tomography.

Aku Seppanen, Antti Lipponen

Department of Applied Physics
University of Eastern Finland
aku.seppanen@uef.fi, antti.lipponen@uef.fi

Jari P. Kaipio
University of Eastern Finland, Finland
University of Auckland, New Zealand
jari@math.auckland.ac.nz

MS40

Variational Approximations in Large-scale Data Assimilation: Experiments with a Quasi-Geostrophic Model

The extended Kalman filter (EKF) is one of the most widely used data assimilation methods. However, EKF is computationally infeasible in large-scale problems, due to the need to store full covariance matrices. Recently, approximations to EKF have been proposed, where the covariance matrices are computed via Limited Memory Broyden-Fletcher-Goldfarb-Shanno (LBFGS) and Conjugate Gradient (CG) optimization methods. In this talk, we review the proposed methods and present data assimilation results using a nonlinear Quasi-Geostrophic benchmark model.

Antti Solonen
Lappeenranta University of Technology
Department of Mathematics and Physics
antti.solonen@gmail.com

MS41

A Spectral Uncertainty Quantification Approach in Ocean General Circulation Modeling

We address the impact of uncertain model parameters on simulations of the oceanic circulation. We focus on high-resolution simulations in Gulf of Mexico during the passage of hurricane Ivan. Uncertainties in subgrid mixing and wind drag parametrizations for HYCOM are propagated using Polynomial Chaos (PC) expansions. A non-intrusive, sparse spectral projection is used to quantify the stochastic model response. A global sensitivity analysis is finally presented that reveals the dominant contributors to prediction uncertainty.

Alen Alexanderian, Justin Winokur, Ihab Sraj
Johns Hopkins University
aalexa20@jhu.edu, jwinokur@jhu.edu, israj1@jhu.edu

Ashwanth Srinivasan
University of Miami
ashwanth@rsmas.miami.edu

Mohamed Iskandarani
Rosenstiel School of Marine and Atmospheric Sciences
University of Miami
MIskandarani@rsmas.miami.edu

WilliamCarlisle Thacker
National Oceanic and Atmospheric Administration
carlisle.thacker@noaa.gov

Omar M. Knio
Duke University
omar.knio@duke.edu

MS41

Uncertainty Quantification of Equation-of-state Closures and Shock Hydrodynamics

We seek to propagate uncertainties in the experimental and numerical atomistic data used to define multiphase equation-of-state (EOS) models to output quantities of interest computed by the equations of shock hydrodynamics. A Bayesian inference approach for characterizing and representing the EOS parametric uncertainty and model discrepancy information is presented. Given the model uncertainty representation, we explicitly demonstrate a viable approach for tabular delivery of uncertain EOS information to the shock hydrodynamics modeling community. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Allen C. Robinson, Robert D. Berry, John H. Carpenter
Sandia National Laboratories
acrobin@sandia.gov, rdberry@sandia.gov,
jhcarpe@sandia.gov

Bert J. Debusschere
Energy Transportation Center
Sandia National Laboratories, Livermore CA
bjdebus@sandia.gov

Richard R. Drake, Ann E. Mattsson
Sandia National Laboratories
rrdrake@sandia.gov, aematts@sandia.gov

William J. Rider
Sandia National Laboratory
wjrider@sandia.gov

MS41

Optimal Uncertainty Quantification and (Non-)Propagation of Uncertainties Across Scales

Posing UQ problems as optimization problems — over infinite-dimensional spaces of probability measures and response functions — gives a method for obtaining sharp bounds on output uncertainties given generic information about input uncertainties. These problems can be solved computationally and sometimes in closed form. Surprisingly, our results show that input uncertainties may fail to propagate across scales if the probabilities and response functions are imperfectly known.

Tim Sullivan, Michael McKerns, Michael Ortiz
California Institute of Technology
tjs@caltech.edu, mmckerns@caltech.edu,
ortiz@aero.caltech.edu

Houman Owhadi
Applied Mathematics
Caltech
owhadi@caltech.edu

Clint Scovel
Los Alamos National Laboratory
jcs@lanl.gov

Florian Theil
University of Warwick
Mathematics Institute

f.theil@warwick.ac.uk

MS41
Coarse Graining with Uncertainty: A Relative Entropy Framework

In this work, we develop a generic framework for uncertainty propagation from an all-atom (AA) system to a coarse-grained (CG) system. The AA system is assumed to follow a probability law that depends on some uncertain parameters. The question we explore is how this uncertainty affects the induced probability law of the CG system. Our solution is posed as a stochastic optimization problem in terms of relative entropies and an efficient solution scheme is developed. The efficacy of the framework is demonstrated numerically.

Nicholas Zabaras
Cornell University
zabaras@cornell.edu

Ilias Bilionis
Center for Applied Mathematics
Cornell University, Ithaca
ib227@cornell.edu

MS42
UQ Practices and Standards for Design and Manufacturing Process Engineering

Design and manufacturing process engineering have always necessitated some degree of uncertainty management. Increasingly complicated systems, with greater performance requirements/constraints, require corresponding advances in uncertainty quantification (UQ) practices. To make effective engineering decisions, these practices are typically implemented with software tools that must address multiple types of uncertainty across a spectrum of models, measurements, and simulations. This talk discusses the present evolution of UQ practices and the potential for improvement through standards development.

Mark Campanelli
National Institute of Standards and Technology
mark.campanelli@nist.gov

MS42
Systematic Integration of Multiple Uncertainty Sources in Design Process

A design optimization methodology is presented that systematically accounts for various sources of uncertainty physical variability (aleatory uncertainty), data uncertainty (epistemic) due to sparse or imprecise data, and model uncertainty (epistemic) due to modeling errors/approximations. A Bayes network approach effectively integrates both aleatory and epistemic uncertainties, and fuses multiple formats of information from models, experiments, expert opinion, and model error estimates. The methodology is illustrated using a three-dimensional wing design problem involving coupled multi-disciplinary simulation.

Sankaran Mahadevan
Vanderbilt University
sankaran.mahadevan@vanderbilt.edu

MS42
Generalized Chapman-Kolmogorov Equation for Multiscale System Analysis

In multiscale system analysis, the effect of incertitude due to lack of knowledge may become significant such that it needs to be quantified separately from inherent randomness. A generalized Chapman-Kolmogorov equation based on generalized interval probability is proposed to describe drift-diffusion and reaction processes under aleatory and epistemic uncertainties. Numerical algorithms are developed to solve the generalized Fokker-Planck equation and interval master equation, where the respective evolutions of the two uncertainty components are distinguished.

Yan Wang
Georgia Institute of Technology
yan.wang@me.gatech.edu

MS43
Macroscopic Properties of Isotropic and Anisotropic Fracture Networks from the Percolation Threshold to Very Large Densities

Some recent studies of fracture networks are summarized. They are made possible by a very versatile numerical technique based on a three-dimensional discrete description of the fractures. Systematic calculations have been made up to very large densities for isotropic, anisotropic networks consisting of fractures distributed according to a power law. The percolation threshold and the macroscopic permeability are shown to be almost independent of the fracture shape when displayed as functions of a dimensionless density calculated by means of the excluded volume.

Pierre Adler
Université Pierre et Marie Curie
France
pierre.adler@upmc.fr

Jean Francois Thovert, Valeri Mourzenko
PPRIME
PPRIME
thovert@icd.ensma.fr, mourzenk@icd.ensma.fr

MS43
Uncertainty Quantification Methods for Unsaturated Flow in Porous Media

We present a stochastic collocation (SC) method to quantify epistemic uncertainty in predictions of unsaturated flow in porous media. SC provides a non-intrusive framework for uncertainty propagation in models based on the non-linear Richards' equation with arbitrary constitutive laws describing soil properties (relative conductivity and retention curve). To illustrate the approach, we use the Richards' equation with the van Genutchen-Mualem model for water retention and relative conductivity to describe infiltration into an initially dry soil whose uncertain parameters are treated as random fields. These parameters are represented using a truncated Karhunen-Lovve expansion; Smolyak algorithm is used to construct a structured set of collocation points from univariate Gauss quadrature rules. A resulting deterministic problem is solved for each collocation point, and together with the collocation weights, the statistics of hydraulic head and infiltration rate are computed. The results are in agreement with Monte Carlo simulations. We demonstrate that highly heterogeneous soils (large variances of hydraulic parameters) require cubature

formulas of high degree of exactness, while their short correlation lengths increase the dimensionality of the problem. Both effects increase the number of collocation points and thus of deterministic problems to solve, affecting the overall computational cost of uncertainty quantification.

David A. Barajas-Solano
Dept. of Mechanical and Aerospace Engineering
University of California, San Diego
d2baraja@ucsd.edu

MS43
A Comparative Study on Reservoir Characterization using Two Phase Flow Model

We consider the problem of characterization of porosity and permeability of reservoir using a two phase flow model. We use a Bayesian MCMC framework to sample these parameters conditioned to available dynamic measurement data. A prefetching procedure to parallelize the MCMC is studied and compared with the multistage MCMC. A set numerical examples are presented to illustrate the comparison.

Victor E. Ginting
Department of Mathematics
University of Wyoming
vginting@uwyo.edu

Felipe Pereira
Center for Fundamentals of Subsurface Flow
University of Wyoming
lpereira@uwyo.edu

Arunasalam Rahunanthan
Center for Fundamentals of Subsurface Flow
University of Wyoming, Laramie, WY 82071
rahu@uwyo.edu

MS43
Adaptive AMG for Diffusion Equations with Stochastic Coefficients

We are interested in solving a 2nd-order diffusion equation where there is uncertainty in the conductivity field. Conditioning conductivity fields to dynamic data using Markov Chain Monte Carlo requires repeated solution of the forward problem for many thousands of realizations of the field. We present an adaptive algebraic multigrid method which automatically adapts to the changing conductivity field in an inexpensive manner. Numerical experiments are discussed for an interesting model problem.

Christian Ketelsen
University of Colorado at Boulder
Ketelsen1@llnl.gov

Panayot Vassilevski
Lawrence Livermore National Laboratory
vassilevski1@linl.gov

MS43
Stochastic Models, Simulation and Analysis in Subsurface Flow and Transport

We discuss stochastic models for heterogeneous random media in the context of numerically computing subsurface flow and transport of fluids. Simulated models are based on series expansions in a variety of bases as well as using geostatistical libraries. The parameterizations employed allow integration of prior observations of the random substrate. Pressures and fluxes are computed numerically and transport curves are compared under different stochastic regimes.

Mina E. Ossiander
Math Dept
Oregon State University
ossiand@math.oregonstate.edu

Malgorzata Peszynska, Veronika S. Vasylkivska
Department of Mathematics
Oregon State University
mpesz@math.oregonstate.edu,
vasylkiv@math.oregonstate.edu

MS44
Spatial Analysis of Energy Consumption by Non-Domestic Buildings in Greater London

This research investigates the influence of local temperatures, building shapes, and mix of buildings across districts on heating energy consumed by non-domestic buildings in London. The goal is to reduce the uncertainty in energy simulation model outputs of buildings by accounting for spatial variations of energy consumption across the city. We explore (and compare) three statistical formulations to quantify the spatial autocorrelations: spatial autoregressive error model, Bayesian geographically weighted regression, and Bayesian CAR model.

Ruchi Choudhary
Department of Engineering
University of Cambridge
rc488@cam.ac.uk

Wei Tian
university of cambridge
wt238@cam.ac.uk

MS44
Spatial Statistical Calibration of a Turbulence Model

The k-ε turbulence model is widely used in CFD modeling. However, it has problems predicting flow separation as well as unconfined and transient flows. We calibrate its parameters against wind tunnel observations of turbulent kinetic energy (TKE) distributed over a two-dimensional cross section of a street canyon. We use a sequential design to pick optimal spatial locations. We then build an emulator to quantify the uncertainty of the modeled TKEs.

Nina Glover, Serge Guillas
University College London
n.glover@ucl.ac.uk, serge@stats.ucl.ac.uk

Liora Malki-Epshtein
UCL
l.malki-epshtein@ucl.ac.uk

MS44
Adding Spatial Dependence Constraints to a Geo-

physical Inverse Problem

Given a geophysical model of seismic pressure wave attenuation, measurements of this attenuation at points in space, and partial information on subsurface soil properties (model parameters), I am interested in estimating the unknown soil properties. This inversion has been done via a stochastic optimization routine because of the complexity of the geophysical model. The goal here is to reduce uncertainty in these estimates by incorporating spatial dependency constraints in the model inversion.

Eugene Morgan
Department of Civil and Environmental Engineering
Duke University
eugene.morgan@duke.edu

MS44

Asessing the Spatial Distribution of Fish Species Using Bayesian Latent Gaussian Models

We describe the use of the integrated nested Laplace approximation (INLA) approach to infer the spatial distribution of fish species, taking into account the spatial autocorrelation, and quantifying the uncertainty. The type of data available (and the methodology used to gather it) will determine the appropriate modelling scheme. In the first example, binary data has been collected that can be regarded as randomly sampled. In the second example, we analyze quantitative data with preferential sampling.

Facundo Muñoz
University of Valencia
facundo.munoz@uv.es

María Pennino
Spanish Institute of Oceanography
grazia.pennino@mu.ieo.es

David Conesa, Antonio López-Quílez
University of Valencia
david.v.conesa@uv.es, antonio.lopez@uv.es

MS45

Uncertainty Quantification for Large Multivariate Spatial Computer Model Output with Climate Applications

Characterizing uncertainty in climate predictions and models is crucial for climate decision-making. One uncertainty source is due to inability to resolve complex physical processes, which is approximated using a parameterization. We characterize parameter uncertainty by calibrating the model to physical observations. Both model output and observations are large multivariate space-time fields. We use Bayesian methods to infer these parameters while incorporating space-time dependence and other uncertainty sources using a Gaussian process emulator and dimension reduction.

K. Sham Bhat
Los Alamos National Laboratory
bhat9999@lanl.gov

MS45

Quantifying Uncertainty for Climate Change Predictions with Model Errorin non-Gaussian Systems

with Intermittency

Synergy between empirical information theory and fluctuation-dissipation theorem provides a systematic framework for improving sensitivity and predictive skill for imperfect models of complex natural systems. We utilize a suite of increasingly complex nonlinear models with intermittent hidden instabilities and time-periodic features to illustrate the advantages of such an approach, as well as the role of model errors due to coarse-graining, moment closure approximations, and the memory of initial conditions in imperfect prediction.

Michal Branicki
New York University
branicki@cims.nyu.edu

Andrew Majda
Courant Institute NYU
jonjon@cims.nyu.edu

MS45

Upper Ocean Singular Vectors of the North Atlantic: Implications for Linear Predictability and Observational Requirement

Recent interest in decadal prediction in the Atlantic sector presumes that the ocean carries sufficient low-frequency predictive skill. We explore the limits of predictability in sea surface temperature and meridional overturning circulation from singular vector calculations with combined tangent linear and adjoint versions of an ocean general circulation model.

Patrick Heimbach
MIT
heimbach@mit.edu

Laure Zanna
Oxford University
zanna@atm.ox.ac.uk

Andrew M. Moore
Univ. of California at Santa Cruz
ammoore@ucsc.edu

Eli Tziperman
Harvard University
eli@seas.harvard.edu

MS45

Quantifying Uncertainties in Fully Coupled Climate Models

Fully coupled climate models are the most realistic tools used to simulate climate change. They incorporate highly detailed, interacting components for the atmosphere, ocean, and sea ice. There is a dire need to quantify their uncertainties, but coupled climate models are computationally very demanding and contain many sources of uncertainty. We describe efforts to quantify uncertainties of the coupled climate system using perturbed-parameter ensembles of the Community Earth System Model.

Scott Brandon, Donald D. Lucas, Curt Covey, Davlid Domyancic, Gardar Johannesson, Stephen Klein, John Tannahill, Yuying Zhang
Lawrence Livermore National Laboratory
brandon1@llnl.gov,   lucas26@llnl.gov,   covey1@llnl.gov,

domyancic1@llnl.gov, johannesson1@llnl.gov, klein21@llnl.gov, tannahill1@llnl.gov, zhang24@llnl.gov

MS46
Efficient Spectral Garlerkin Method with Orthogonal Polynomials for SPDES

In this talk we first develop a fast algorithm to evaluate orthogonal polynomial expansions for d-variable functions in on sparse grids. Then we apply this fast algorithm to develop an efficient spectral method to approximate the solutions of stochastic partial differential equations with random input data. Three aspects distinguishes work from the existing ones: 1. Our algorithm is applicable L^2 functions with arbitrary probability density weight; 2. The use of orthogonal polynomials results in matrix sparsity; 3. Exponential rate of convergence of the numerical algorithm is rigorously proved.

Yanzhao Cao
Department of Mathematics & Statistics
Auburn University
yzc0009@auburn.edu

MS46
Adaptive Methods for Elliptic Partial Differential Equations with Random Operators

Solutions of random elliptic boundary value problems admit efficient approximations by polynomials on the parameter domain, but it is not clear a priori which polynomials are most significant. I will present numerical methods that adaptively construct suitable spaces of polynomials. These methods are based on adaptive finite elements and adaptive wavelet algorithms, with orthonormal polynomial systems in place of wavelet bases. They construct efficient sparse representations of the approximate solution.

Claude Gittelson
Purdue University
cgittels@purdue.edu

MS46
Efficient Nonlinear Filtering of a Singularly Perturbed Stochastic Hybrid System

Astract not available at time of publication.

Boris Rozovski
Brown University
boris_rozovsky@brown.edu

MS46
Two Stochastic Modeling Strategies for Elliptic Problems

In this talk, we compare two stochastic elliptic models: $-\nabla \cdot (a(x,\omega) \cdot \nabla u(x,\omega)) = f(x)$ and $-\nabla \cdot \left(\left(a^{-1}\right)^{\diamond(-1)} \diamond \nabla u(x,\omega) \right) = f(x)$, where $a(x,\omega)$ is a log-normal random field, with respect to the two characteristic parameters of the underlying Gaussian random field, i.e., the standard deviation and the correlation length. Some related numerical issues and numerical results will be discussed.

Xiaoliang Wan
Louisiana State University
Department of Mathematics
xlwan@math.lsu.edu

MS47
Putting Computational Inference into an FPGA

We are building a compiler to map large numerical computations into FPGAs (Field Programmable Gate Array). Our target application is MCMC (Markov chain Monte Carlo) based inference for ECT (Electrical Capacitance Tomography). We aim to realize the good compute throughput of FPGAs, both in terms of performance-per-dollar and performance-per-Watt, to perform real-time UQ embedded into industrial sensors.

Colin Fox
University of Otago, New Zealand
fox@physics.otago.ac.nz

MS47
Model Reductions by MCMC

Identification of models is often complicated by the fact that the available experimental data from field measurements is noisy or incomplete. Moreover, models may be complex, and contain a large number of correlated parameters. As a result, the parameters are poorly identified by the data, and the reliability of the model predictions is questionable. We consider a general scheme for reduction and identification of dynamic models using two modern approaches, Markov chain Monte Carlo sampling methods together with asymptotic model reduction techniques. The ideas are illustrated with examples related to bio-medical applications and epidemiology.

Heikki Haario
Lappeenranta University of Technology
Department of Mathematics and Physics
heikki.haario@lut.fi

MS47
Advanced Uncertainty Evaluation of Climate Models by Monte Carlo Methods

Uncertainties in future climate projections are often evaluated based on the perceived spread of ensembles of multimodel climate projections. Here we focus on the uncertainties related to a single climate model and its closure parameters that are used in physical parameterization schemes and cover topics such as specification of the cost function and parameter identification by Monte Carlo methods.

Marko Laine
Finnish Meteorological Institute
marko.laine@fmi.fi

MS47
Covariance Estimation Using Chi-squared Tests

Regularized solutions of ill-posed inverse problems can be viewed as solutions of the original problem when the problem is regularized by adding statistical information to it. The discrepancy principle finds a regularization parameter by applying a chi-square test, and we extend and improve the approach to estimate a regularization matrix. This regularization matrix can be viewed as an estimate of an error covariance matrix. Results will be shown from an

event reconstruction problem.

Jodi Mead
Boise State University
Department of Mathematics
jmead@boisestate.edu

MS48
Heterogeneous Deformation of Polycrystalline Metals and Extreme Value Events

Astract not available at time of publication.

Curt Bronkhorst
Los Alamos National Lab
cabronk@lanl.gov

MS48
Coupled Chemical Master Equation - Fokker Planck Solver for Stochastic Reaction Networks

Stochastic reaction networks are generally governed by the Chemical Master Equation (CME). While the CME, as a high-dimensional ODE system, is hard to solve in general, its continuum approximations, e.g. Focker-Planck equations (FPE), are reliable alternatives when the species count is large enough. We present a proof-of-concept methodology for a hybrid construction that effectively combines CME and FPE, employing a discrete scale CME solution in regions where the continuum FPE is inaccurate.

Khachik Sargsyan, Cosmin Safta
Sandia National Laboratories
ksargsy@sandia.gov, csafta@sandia.gov

Bert J. Debusschere
Energy Transportation Center
Sandia National Laboratories, Livermore CA
bjdebus@sandia.gov

Habib N. Najm
Sandia National Laboratories
Livermore, CA, USA
hnnajm@sandia.gov

MS48
A New Approach for Solving Multiscale SPDEs using Probabilistic Graphical Models

We propose a hierarchical representation of random fields by capturing the stochastic input at fine scale with locally reduced models and combining them with graphical models on the coarse scale. Regression models are constructed such that local features are taken as input and multiscale basis functions as output. In this way, we can make samples of coarse scale properties from the graphical probabilistic model, obtain multiscale basis functions with regression models and solve SPDEs on the coarse scale.

Nicholas Zabaras
Cornell University
zabaras@cornell.edu

Jiang Wan
Corness University
jw688@cornell.edu

MS49
A Reduced Order Model for a Nonlinear, Parameterized Heat Transfer Test Case

We present a reduced order model (ROM) for heat transfer through a composite fiber with two material properties. The ROM is constructed by interpolating the components of a modal decomposition (SVD) of a sampling of high-fidelity models – each computed with different material properties. We are able to scale the SVD using a novel implementation in MapReduce. We then use the ROM as a cheap surrogate to study the probability of failure of the system.

Paul Constantine, Jeremy Templeton
Sandia Labs
paulcon@stanford.edu, n/a

Joe Ruthruff
Livermore
n/a

MS49
Uncertainty Quantification for Turbulent Mixing and Turbulent Combustion

Large eddy simulations of mixing and combustion with finite rate chemistry eliminate a major source of chemistry model related (epistemic)uncertainty. The method is a notion of stochastic convergence, to generate space-time dependent PDFs (Young's measures) out of a single simulation via coarse graining with the multiple mesh values in a supercell to generate the PDF. Comparison to experimental data related to a Scram jet is included. Comparison to RANS and other simulations allows model related error assessment and uncertainty quantification.

James G. Glimm
Stony Brook University
Brookhaven National Laboratory
glimm@ams.sunysb.edu or glimm@bnl.gov

MS49
Chemical Kinetic Uncertainty Quantification for High-Fidelity Turbulent Combustion Simulations

Detailed chemical mechanisms consist of hundreds or thousands of chemical reactions with an uncertain rate for each. Direct propagation of this very high-dimensional uncertainty through high-fidelity Large Eddy Simulation (LES) of turbulent reacting flows is computationally intractable. Instead, a method is presented in which the pre-processing portion of the turbulent combustion model is used to condition this very high-dimensional uncertainty, resulting in a lower-dimensional uncertainty space that is efficiently propagated through the LES. The approach is demonstrated with a laboratory-scale turbulent nonpremixed jet flame.

Michael Mueller
Stanford
muellerm@stanford.edu

Gianluca Iaccarino
Stanford University
jops@stanford.edu

Heinz Pitsch
Stanford

na/

MS49
Criteria for Optimization Under Uncertainty

In this work different criteria for robust optimization under uncertainty are compared. In particular, a framework proposed by the authors and characterized by the use of all the possible information in the probabilistic domain, namely the Cumulative Distribution Function (CDF), is compared to more classical approaches that rely on the usage of classical statistical moments as deterministic attributes that define the objectives of the optimization process. Furthermore, the use of an area metric leads to a multi-objective methodology which allows an a posteriori selection of the candidate design based on risk/opportunity criteria defined by the designer. A comparison with another new technique based on Evidence Theory, proposed by different authors, is also introduced.

Domenico Quagliarella
Centro Italiano Ricerche Aerospaziali
d.quagliarella@cira.it

G. Petrone
University Federico II of Naples
gpetrone@stanford.edu

Gianluca Iaccarino
Stanford University
jops@stanford.edu

MS50
Bayesian Uncertainty Quantification for Flows in Highly Heterogeneous Media

Abstract not available at time of publication.

Yalchin Efendiev
Dept of Mathematics
Texas A&M University
efendiev@math.tamu.edu

MS50
Emulators in Large-scale Spatial Inverse Problems

We consider a Bayesian approach to nonlinear inverse problems in which the unknown quantity (input) is a random field (spatial or temporal). The forward model is complex and non linear, therefore computationally expensive. We develop an emulator based approach where the Bayesian multivariate adaptive splines (BMARS) has been used to model unknown functions of the model input. We consider discrete cosine transformation (DCT) for dimension reduction of the input field. The estimation is carried out using trans dimensional Markov chain Monte Carlo. Numerical results are presented by analyzing simulated as well as real data for reservoir characterization.

Anirban Mondal
Quantum Reservoir Impact
anirban.mondal@qrigroup.com

MS50
Uncertainty Quantification for Reactive Transport of Contaminants

The fate and transport of contaminants in the subsurface is strongly influenced by bio-geochemical reactions. Predictions are routinely compromised by both model (structural) and parametric uncertainties. I will first present a set of computational tools for quantifying these two types of uncertainties for multi-component nonlinear chemical reactions. The second part of the talk will deal with the combined effects of uncertainty in reactions and heterogeneity of the medium on the transport of reactive contaminants.

Gowri Srinivasan
T-5, Theoretical Division, Los Alamos National
Laboratory
gowri@lanl.gov

MS50
A Framework for Experimental Design for Ill-posed Inverse Problems

A fremework for experimental design for ill-posed inverse problems We consider the problem of experimental design for ill-posed inverse problems. The main difficulties we have to address are: the bias introduced by the regularization of the inverse problem, and the parameter selection required by the regularization. We propose a Bayesian approach based on a hierarchical sequence of prior moment conditions. The methodology applies also to a non-Bayesian mathod based on training models. We provide generalization of the usual equivalence theorems and propose numerical methods to tackle large-scale problems.

Luis Tenorio
Colorado School of Mines
ltenorio@mines.edu

MS51
An Approach for the Adaptive Solution of Optimization Problems Governed by PDEs with Uncertain Coefficients

Using derivative based numerical optimization routines to solve optimization problems governed by partial differential equations (PDE) with uncertain coefficients is computationally expensive due to the large number of PDE solves required at each iteration. I propose a framework for the adaptive solution of such optimization problems based on the retrospective trust region algorithm. I prove global convergence of the retrospective trust region algorithm under weak assumptions on gradient inexactness. If one can bound the error between actual and modeled gradients using reliable and efficient a posteriori error estimators, then the global convergence of the proposed algorithm follows. I present a stochastic collocation finite element method for the solution of the PDE constrained optimization. In the stochastic collocation framework, the state and adjoint equations can be solved in parallel. Initial numerical results for the adaptive solution of these optimization problems are presented.

Drew Kouri
Department of Computational and Applied Mathematics
Rice University
drew.kouri@rice.edu

MS51
Uncertainty Quantification using Nonparametric

Estimation and Epi-Splines

We address uncertainty quantification in complex systems by a flexible, nonparametric framework for estimation of density and performance functions. The framework systematically incorporates hard information derived from physics-based sensors, field test data, and computer simulations as well as soft information from human sources and experiences. The framework is based on epi-splines for consistent approximation of infinite-dimensional optimization problems arising in the estimation process. Preliminary numerical results indicate that the framework is highly promising.

Johannes O. Royset
Asst. Prof.
Naval Postgraduate School
joroyset@nps.edu

Roger Wets
University of California, Davis
rjbwets@ucdavis.edu

MS51

Numerical Methods for Shape Optimization under Uncertainty

The proper treatment of uncertainties in the context of aerodynamic shape optimization is a very important challenge to ensure a robust performance of the optimized airfoil under real life conditions. This talk will propose a general framework to identify, quantize and include stochastic distributed, aleatory uncertainties in the overall optimization procedure. Appropriate robust formulations of the underlying deterministic problem and uncertainty quantification techniques in combination with adaptive discretization approaches are investigated in order to measure the effects of the uncertainties in the input data on quantities of interest in the output. Finally, algorithmic approaches based on multiple-setpoint ideas in combination with one-shot methods as well as numerical results are presented.

Claudia Schillings
University of Trier, Germany
Claudia.Schillings@uni-trier.de

Volker Schulz
University of Trier
Department of Mathematics
Volker.Schulz@uni-trier.de

MS51

Risk Neutrality and Risk Aversion in Shape Optimization with Uncertain Loading

Conceptually inspired by finite-dimensional stochastic programming with recourse we propose infinite-dimensional two-stage stochastic models for shape optimization of elastic bodies with linearized elasticity and stochastic loading. Risk neutral and risk averse approaches, the latter involving suitable risk measures or dominance relations, will be discussed. Reporting illustrative computational experiments concludes the talk.

Ruediger Schultz
University of Duisburg-Essen
ruediger.schultz@uni-due.de

MS52

Spatial ANOVA Modeling of High-resolution Regional Climate Model Outputs from NARCCAP

The differences between future (2041-2070) and current (1971-2000) average seasonal temperature fields, from two regional climate models (RCMs) driven by the same atmosphere-ocean general circulation model in the North American Regional Climate Change Assessment Program (NARCCAP), are analyzed using a hierarchical two-way ANOVA model with the factors of season, RCM, and their interaction. The spatial variability across the domain is modeled through the Spatial Random Effects (SRE) model, which allows for efficient computation.

Emily L. Kang
Department of Mathematical Sciences
University of Cincinnati
kangel@ucmail.uc.edu

Noel Cressie
Ohio State University
ncressie@stat.osu.edu

MS52

Statistical Issues in Catchment Scale Hydrological Modeling

Many uncertainty quantification methods currently in use by the hydrological community make the mistake of implicitly conflating the hydrological model with the true physical system. Rather than using a framework with an additive discrepancy term, I will argue for making the hydrological model itself stochastic, expressed using a system of stochastic differential equations. I will discuss Bayesian inference under this model, which falls under the difficult category of dynamic models with non-time-varying parameters.

Cari Kaufman
University of California, Berkeley
cgk@stat.berkeley.edu

MS52

Quantifying Uncertainties in Hydrologic Parameters in the Community Land Model

Uncertainties in hydrologic parameters could have significant impacts on the simulated water and energy fluxes and land surface state, which can affect carbon cycle and atmospheric processes in coupled earth system simulations. In this study, we introduce an uncertainty quantification (UQ) framework for sensitivity analyses and uncertainty quantification of selected parameters related to hydrologic processes in the Community Land Model. Ten flux tower sites and over fifteen watersheds spanning a wide range of climate and site conditions were selected to perform sensitivity analyses by perturbing the parameters identified. An Entropy-based approach was used to derive prior PDF for each input parameter and the Quasi-Monte Carlo (QMC) approach was used to generate samples of parameters from the prior PDFs. A simulation for each set of sampled parameters was performed to obtain response curves. Based on statistical tests, the parameters were ranked for their significance depending on the simulated latent heat flux, sensible heat flux, and total runoff. The study provides the basis for parameter dimension reduction and guidance on parameter calibration framework design, under different

hydrologic and climatic regimes.

Ruby Leung
Pacific Northwest National Laboratory
ruby.leung@pnnl.gov

Zhangshuan Hou, Maoyi Huang, Yinghai Ke
Pacific Northwest National Lab
zhangshuan.hou@pnnl.gov, maoyi.huang@pnnl.gov,
yinghai.ke@pnnl.gov

Guang Lin
Pacific Northwest National Laboratory
guang.lin@pnnl.gov

MS52
Uncertainty Propagation in Land-Crop Models

Crop models were recently included in the land model of the Community Earth System Model (CESM). Good estimates of physiology parameters for crops are essential to get accurate outputs, particularly carbon cycle ones. To that end, we investigate the potential of intrusive uncertainty quantity approaches when used in combination with maximum likelihood/ regression models for calibrating the crop model parameters from Ameriflux data. Numerical tests for this approach using soybean data from the Bondville, IL site produced very promising initial results.

Xiaoyan Zeng
Argonne National Laboratory
zeng@mcs.anl.gov

Mihai Anitescu, Emil M. Constantinescu
Argonne National Laboratory
Mathematics and Computer Science Division
anitescu@mcs.anl.gov, emconsta@mcs.anl.gov

MS53
Basis and Measure Adaptation for Stochastic Galerkin Projections

Use of the stochastic Galerkin finite element methods leads to large systems of linear equations.These systems are typically solved iteratively.We propose a preconditioner which takes advantage of the recursive hierarchy in the structure of the global system matrices. Neither the global matrix, nor the preconditioner need to be formed explicitly.The ingredients include only the number of stiffness matrices from the truncated Karhunen-Loève expansion and a preconditioner for the mean-value problem.The performance is illustrated by numerical experiments.

Roger Ghanem
University of Southern California
Aerospace and Mechanical Engineering and Civil
Engineering
ghanem@usc.edu

Bedřich Sousedík
University of Southern California
bedrich.sousedik@gmail.com

Eric Phipps
Sandia National Laboratories
Optimization and Uncertainty Quantification Department
etphipp@sandia.gov

MS53
A Stochastic Collocation Method Based on Sparse Grid for Stokes-Darcy Model with Random Hydraulic Conductivity

The Stokes-Darcy model has attracted significant attention since its higher fidelity than either Darcy or Stokes system is important for many applications, but uncertainties and coupling issues lead to a rather complex system. We present a stochastic collocation method based on sparse grid for the Stokes-Darcy model with random hydraulic conductivity. This method is natural for parallel computation and some numerical results are presented to illustrate the features of this method.

Max Gunzburger
Florida State University
School for Computational Sciences
mgunzburger@fsu.edu

Xiaoming He, Xuerong Wen
Department of Mathematics and Statistics
Missouri University of Science and Technology
hex@mst.edu, wenx@mst.edu

MS53
Adaptive Sparse Grid Generalized Stochastic Collocation Using Wavelets

Accurate predictive simulations of complex real world applications require numerical approximations to first, oppose the *curse of dimensionality* and second, converge quickly in the presence of steep gradients, sharp transitions, bifurcations or finite discontinuities in high-dimensional parameter spaces. In this talk we present a novel multidimensional multiresolution adaptive (MdMrA) sparse grid stochastic collocation method, that utilizes hierarchical multiscale piecewise Riesz basis functions constructed from interpolating wavelets. The basis for our non-intrusive method forms a stable multiscale splitting and thus, optimal adaptation is achieved. Error estimates and numerical examples will used to compare the efficiency of the method with several other techniques.

Clayton G. Webster
Oak Ridge National Laboratory
webstercg@ornl.gov

Max Gunzburger
Florida State University
School for Computational Sciences
mgunzburger@fsu.edu

John Burkardt
Department of Computational Science
Florida State University
jburkardt@fsu.edu

MS53
Error Analysis of a Stochastic Collocation Method for Parabolic Partial Differential Equations with Random Input Data

A stochastic collocation method for solving linear parabolic PDEs with random input data is analyzed. The input data are assumed to depend on a finite number of random variables. Unlike previous analysis, a wider range of situations is considered including input data that depend nonlinearly on the random variables and random variables that are

correlated or even unbounded. We demonstrate exponential convergence of the interpolation error for both a semi-discrete and a fully-discrete scheme.

Guannan Zhang
Florida State University
gzhang5@fsu.edu

Max Gunzburger
Florida State University
School for Computational Sciences
mgunzburger@fsu.edu

MS54
Retrospective-Cost-Based Model Refinement of Systems with Inaccessible Subsystems

Spatially discretized models are typically constructed based on physical laws and parameter estimates. These models may be erroneous, however, due to unmodeled physics and numerical errors. These discrepancies become apparent when model predictions disagree with measurements. The goal of this research is to use data to improve the fidelity of an initial model. The approach we take is based on retrospective-cost-based optimization of subsystems that are inaccessible, that is, whose inputs and outputs are not measured. Applications to space weather modeling will be presented.

Dennis Bernstein
University of Michigan
dsbaero@umich.edu

Anthony D'Amato, Asad Ali
Aerospace Engineering Department
University of Michigan
amdamato@umich.edu, asadali

MS54
Multiscale Methods for Flows in Heterogeneous Stochastic Porous Media

In this talk, I will discuss multiscale methods for stochastic problems. The main idea of our approach is to construct local basis functions that encode the local features present in the coefficient to approximate the solution of parameter-dependent flow equation. Constructing local basis functions involves (1) finding initial multiscale basis functions and (2) constructing local spectral problems for complementing the initial coarse space. We use the Reduced Basis (RB) approach to construct a reduced dimensional local approximation that allows quickly computing the local spectral problem. I will present the details of the algorithm, numerical results, and computational cost. Applications to Bayesian Uncertainty Quantification will be discussed. This is a joint work with Juan Galvis (TAMU) and Florian Thomines (ENPC).

Yalchin Efendiev
Dept of Mathematics
Texas A&M University
efendiev@math.tamu.edu

MS54
Feedback Particle Filter: A New Formulation for Nonlinear Filtering Based on Mean-field Games

A new formulation of the particle filter for nonlinear filtering is presented, based on concepts from optimal control, and from mean-field game theory. The feedback particle filter admits an innovations error-based feedback control structure: The control is chosen so that the posterior distribution of any particle matches the posterior distribution of the true state given the observations. The feedback particle filter is shown to have significant advantages over the conventional particle filter in the numerical examples considered. Application to Bayesian inference in neural circuits is briefly discussed with the aid of coupled oscillator models.

Tao Yang
UIUC
taoyang1@illinois.edu

Prashant G. Mehta
Department of Mechanical and Industrial Engineering
University of Illinois at Urbana Champaign
mehtapg@uiuc.edu

Sean Meyn
Department of Electrical and Computer Engineering
University of Illinois at Urbana Champaign
meyn@illinois.edu

MS54
Uncertainty Analysis of Dynamical Systems – Application to Volcanic Ash Transport

Uncertainty analysis of a number of societally important physical systems may be posed in the dynamic systems framework. In this leadoff talk we will overview this minisymposium on this topic and frame issues using our group's work on transport of volcanic ash transport. Basic approaches and results of application of these methods to recent eruption events will be presented.

Abani K. Patra
SUNY at Buffalo
Dept of Mechanical Engineering
abani@eng.buffalo.edu

Puneet Singla
Mechanical & Aerospace Engineering
University at Buffalo
p.singla@gmail.com

Marcus Bursik
Dept. of Geology
SUNY at Buffalo
mib@buffalo.edu

E. Bruce Pitman
Dept. of Mathematics
Univ at Buffalo
pitman@buffalo.edu

Matthew Jones
Center for Comp. Research,
Univ. at Buffalo, Buffalo, NY 14260
jonesm@buffalo.edu

Tarunraj Singh
Dept of Mechanical Engineering
SUNY at Buffalo
tsingh@buffalo.edu

MS55

Optimal Use of Gradient Information in Uncertainty Quantification

We discuss methods that use derivative information for probabilistic uncertainty propagation in models of complex system. We demonstrate that such methods needs less sampling information compared to their derivative-free version. Here we discuss the importance of several algorithmic choices, such as the choice of basis in regression with derivative information, the choice of error model by means of Gaussian processes, and the choice of sampling points based on optimal design considerations. We demonstrate in particular that standard choices originating from derivative-free methods are not suitable in this circumstance, and we define criteria adapted to the use of derivative information that result in novel designs and bases. We demonstrate our findings on models from nuclear engineering.

Mihai Anitescu
Argonne National Laboratory
Mathematics and Computer Science Division
anitescu@mcs.anl.gov

Fred J. Hickernell
Illinois Institute of Technology
Department of Applied Mathematics
hickernell@iit.edu

Yiou Li
Illinois Institute of Technology
yli88@stuart.iit.edu

Oleg Roderick
Argonne National Laboratory
roderick@mcs.anl.gov

MS55

Gradient-based Optimization for Mixed Epistemic and Aleatory Uncertainty

Within this talk, a novel sampling/optimization approach to mixed aleatory/epistemic uncertainty quantification is presented for hypersonic computational fluid dynamic simulations. This approach uses optimization to propagate epistemic uncertainty to simulation results while sampling of these optimization results is used to characterize the distribution due to aleatory variables. To reduce the required number of optimizations, a Kriging surrogate is employed. For this talk, this combined sampling/optimization approach will be demonstrated for analytic functions and simulations drawn from hypersonic fluid flows. Additionally, the performance of a similar uncertain optimization approach is tested for this application.

Brian Lockwood
University of Wyoming
blockwoo@uwyo.edu

Dimitri Mavriplis
Department of Mechanical Engineering
University of Wyoming
mavripl@uwyo.edu

MS55

Gradient-based Data Assimilation in Atmospheric

Applications

Adaptivity in space and time is ubiquitous in modern numerical simulations. To date, there is still a considerable gap between the stateoftheart techniques used in direct (forward) simulations, and those employed in the solution of inverse problems, which have traditionally relied on fixed meshes and time steps. This talk describes a framework for building a space-time consistent adjoint discretization for a general discrete forward problem, in the context of adaptive mesh, adaptive time step models.

Adrian Sandu
Virginia Polytechnic Institute and
State University
sandu@cs.vt.edu

Mihai Alexe
Virginia Tech
Department of Computer Science
mihai@vt.edu

MS55

Sensitivity Analysis and Error Estimation for Differential Algebraic Equations in Nuclear Reactor Applications

We develop a general framework for computing the adjoint variable to nuclear engineering problems governed by a set of differential-algebraic equations. We use an abstract variational approach to develop the framework, which provides flexibility in modification and expansion of the governing equations. Using both a simplex example with known solution and a dynamic reactor model, we show both theoretically and numerically that the framework can be used for both parametric uncertainty quantification and the estimation of global time discretization error.

Hayes Stripling
Texas A&M University
Nuclear Engineering Department
h.stripling@tamu.edu

Mihai Anitescu
Argonne National Laboratory
Mathematics and Computer Science Division
anitescu@mcs.anl.gov

Marvin Adams
Texas A&M University
mladams@ne.tamu.edu

MS56

A Semi-Intrusive Deterministic Approach to Uncertainty Quantifications

This paper deals with the formulation of a semi-intrusive (SI) method allowing the computation of statistics of linear and non linear PDEs solutions. This method shows to be very efficient to deal with probability density function of whatsoever form, long-term integration and discontinuities in stochastic space. The effectiveness of this method is illustrated for a modified version of Kraichnan-Orszag three-mode problem where a discontinous pdf is associated to the stochastic variable, and for a nozzle flow with shocks. The results have been analyzed in terms of accuracy and probability measure flexibility. Finally, the importance of the probabilistic reconstruction in the stochastic space is shown up on an example where the exact solution is com-

putable, in the resolution of the viscous Burgers equations. We expect some more applications by the time of the conference.

Remi Abgrall
INRIA Bordeaux Sud-Ouest
Universite de Bordeaux
remi.abgrall@inria.fr

James G. Glimm
Stony Brook University
Brookhaven National Laboratory
glimm@ams.sunysb.edu or glimm@bnl.gov

MS56
Uncertainty Quantification with Incomplete Physical Models

The emergence of uncertainty quantification (UQ) has been a critical development towards the goal of predictive science. The many efficient, non-intrusive, intuitive approaches of probabilistic uncertainty have accelerated the widespread adoption of the methodology. The additional uncertainty arising from incomplete physical models makes the analysis much less obvious. This work examines how optimization over a restricted class of functionals can bound the analysis of the true model if it were available. Furthermore, these bounds provide insight into the sensitivity of this knowledge-gap relative to the overall prediction.

Gianluca Iaccarino
Stanford University
jops@stanford.edu

Gary Tang
Stanford
garytang@stanford.edu

MS56
Numerical Methods for Polynomial Chaos in Uncertain Flow Problems

The Euler equations subject to input uncertainty are investigated via the stochastic Galerkin approach. We present a fully intrusive method based on a variable transformation of the continuous equations. Roe variables are employed to get quadratic dependence in the flux function. The Roe formulation saves computational cost compared to the formulation based on expansion of conservative variables, and can handle cases of supersonic flow, for which the conservative variable formulation leads to instability.

Mass Per Pettersson
Stanford University
massperp@stanford.edu

MS56
Evidence Based Multiciplinary Robust Design

Abstract not available at time of publication.

Massimilian Vasile
University of Strathclyde
m.vasile@aero.gla.ac.uk

MS57
Toward Estimation of Sub-ice Shelf Melt Rates to Ocean Circulation Under Pine Island Ice Shelf, West Antarctica

Increased melt rates under ice shelves around Antarctica have been suggested as a dominant cause for observed acceleration of the ice sheet near its marine margin. The melt rates are difficult to observe directly. We present first steps towards estimating the melt rates from accessible hydrography and optimal control methods. We address to which extent hydrographic observations away from the ice-ocean boundary can be used to constrain melt rates. We derive sensitivity patterns of melt rates to changes in ocean circulation underneath the Pine Island Ice-Shelf. The sensitivity patterns are computed with an adjoint model of an ocean general circulation model that resolves the sub-ice shelf circulation. Inverting for best-estimate melt rates presents a first step towards backward propagation of uncertainties.

Patrick Heimbach
MIT
heimbach@mit.edu

Martin Losch
Alfred Wegener Institute
martin.losch@awi.de

MS57
Ice Bed Geometry: Estimates of Known Unknowns

For ice sheets, kilometer scale features in bed geometry may dominate scenarios of ice mass loss. We developed a radar sensor model for Thwaites basin in West Antarctica and use conditional simulations of off-track features to characterize unknown knowns of its bed geometry. We shall discuss the observational, scientific, and statistical strategies for quantifying effects of bed geometry uncertainties on estimates of sea level rise.

Charles Jackson
UTIG
University of Texas at Austin
charles@ig.utexas.edu

Chad Greene
Department of Geological Sciences
The University of Texas at Austin
chad allen greene ¡chadagreene@utexas.edu¿

John Goff, Scott Kempf, Duncan Young
Institute for Geophysics
The University of Texas at Austin
goff@ig.utexas.edu, scottk@ig.utexas.edu,
young@ig.utexas.edu

Evelyn Powell
Institute for Geophysics
evelyn powell ¡empressofme@gmail.com¿

Don Blankenship
UTIG
University of Texas at Austin
blank@ig.utexas.edu

MS57
Quantification of the Uncertainty in the Basal Slid-

ing Coefficient in Ice Sheet Models

The estimation of uncertainty in the solution of ice sheet inverse problems within the framework of Bayesian inference is considered. We exploit the fact that for Gaussian noise and prior probability densities and linearized parameter-to-observable map the posterior density (i.e., the solution of the statistical inverse problem) is Gaussian and hence is characterized by its mean and covariance. The method is applied to quantify uncertainties in the inference of basal boundary conditions for ice sheet models.

Noemi Petra
Institute for Computational Engineering and Sciences
University of Texas at Austin
noemi@ices.utexas.edu

Hongyu Zhu
Institute for Computational Engineering and Sciences
The University of Texas at Austin
zhuhongyu@ices.utexas.edu

Georg Stadler, Omar Ghattas
University of Texas at Austin
georgst@ices.utexas.edu, omar@ices.utexas.edu

MS57

Bayesian Calibration via Additive Regression Trees with Application to the Community Ice Sheet Model

Quantifying uncertainties in calibration experiments involving complex computer models with high dimensional input spaces and large outputs is often infeasible. We develop a non-parametric Bayesian trees model that scales to challenging calibration problems. Here, each tree represents a weak learner and the overall model is a sum-of-trees. The idea is to learn locally-adaptive bases while retaining efficient MCMC sampling of the posterior distribution. We demonstrate our method by calibrating the Community Ice Sheet Model.

Matthew Pratola, Stephen Price, David Higdon
Los Alamos National Laboratory
mpratola@lanl.gov, sprice@lanl.gov, dhigdon@lanl.gov

MS58

Reduced Basis, the Discrete Interpolation Method and Fast Quadratures for Gravitational Waves

Finding gravitational waveforms (GWs) is potentially going to open a new window to the universe. Einstein's equations are nonlinear parameter dependent (mass, spin etc.) PDEs that approximate the post-Newtonian equations (PN). PN without spin gives stationary phase approximations (SPA) to waveforms. Using matched filtering techniques, a LIGO search to find GWs, requires about 10,000 SPA templates and several months on supercomputers. Reduced basis and using DEIM points as quadrature nodes leads to significant savings.

Harbir Antil
The University of Maryland
hantil@math.umd.edu

MS58

Decreasing the Temporal Complexity in Nonlinear

Model Reduction

UQ for nonlinear dynamical systems presents a challenge: uncertainty-space sampling requires thousands of large-scale simulations. To mitigate this burden, researchers have developed model-reduction techniques that decrease the model's 'spatial complexity' by decreasing 1) the number of degrees of freedom and 2) the complexity of nonlinear functions evaluations. However, when an implict time integrator is used, the number of time steps remains very large. This talk presents a strategy for decreasing the model's 'temporal complexity'.

Kevin T. Carlberg
Stanford University
ktcarlb@sandia.gov

MS58

Error Analysis for Nonlinear Model Reduction Using Discrete Empirical Interpolation in the Proper Orthogonal Decomposition Approach

Discrete Empirical Interpolation Method (DEIM) is an efficient technique for resolving the complexity issue of the standard projection-based model reduction methods, such as the popular Proper Orthogonal Decomposition (POD) approach, due to nonlinearities of dynamical systems. Recently, the hybrid approach combining POD with DEIM has been successfully used to obtain accurate low-complexity reduced systems in many applications. However, error analysis for this approach has not been investigated yet. This work provides state space error bounds for the solutions of reduced systems constructed from this POD-DEIM approach. The analysis is particularly relevant to ODE systems arising from spatial discretizations of parabolic PDEs. The resulting error bounds reflect the POD approximation property through the decay of singular values, as well as explain how the DEIM approximation error involving the nonlinear term comes into play. The conditions under which the stability of the original system is preserved and the reduction error is uniformly bounded will be discussed.

Saifon Chaturantabut
Virginia Tech
saifonc@math.vt.edu

Danny C. Sorensen
Rice University
sorensen@rice.edu

MS58

Linearized Reduced-order Models for Optimization and Data Assimilation in Subsurface Flow

Trajectory piecewise linearization (TPWL) is a reduced-order modeling approach where new solutions for nonlinear problems are represented using linear expansions around previously simulated (and saved) solutions. The high-dimensional representation is projected into a low-dimensional subspace using proper orthogonal decomposition, which results in very large runtime speedups. We describe the application of TPWL for the optimization of well settings in oil reservoir simulation and for inverse problems involving the determination of geological parameters.

Jincong He
Stanford University
jincong@stanford.edu

Lou J. Durlofsky
Stanford University
Dept of Petroleum Engineering
lou@stanford.edu

MS59
Testbeds for Ocean Model Calibration

Tuning and uncertainty quantification in ocean models is challenging particularly because of the lack of suitable observation datasets, and the computational expense in running full-Earth simulations. Ocean models can be run in limited instances at an eddy-resolving resolution, so high-resolution runs can be a target response for lower-resolution parameterization. Testbed configurations are then sufficient to expose effects of concern. We show results from a channel model representative of the Antarctic Circumpolar Current (ACC), emphasizing eddy heat transport.

James Gattiker, Matthew Hecht
Los Alamos National Laboratory
gatt@lanl.gov, mhecht@lanl.gov

MS59
An Overview of Uncertainty Quantification in the Community Land Model

The Community Land Model (CLM) is the terrestrial component of the Community Earth System Model (CESM), which is used extensively for projections of the future climate system. CLM has over 100 uncertain parameters, contains multiple nonlinear feedbacks, and is computationally demanding, presenting a number of challenges for UQ efforts. CLM modeling has benefitted from our initial UQ efforts through a new ability to rank parameters by relative importance and to identify unrealistic parameter combinations.

Daniel Ricciuto, Dali Wang
Oak Ridge National Laboratory
ricciutodm@ornl.gov, wangd@ornl.gov

Cosmin Safta, Khachik Sargsyan
Sandia National Laboratories
csafta@sandia.gov, ksargsy@sandia.gov

Habib N. Najm
Sandia National Laboratories
Livermore, CA, USA
hnnajm@sandia.gov

Peter Thornton
Oak Ridge National Laboratory
thorntonpe@ornl.gov

MS59
Efficient Surrogate Construction for High-Dimensional Climate Models

In this study we explore the use of non-intrusive methods to construct surrogate approximations for the Community Land Model (CLM). Relevant vector machine techniques are used to reduce the dimensionality of the input space. This approach is used in conjunction with adaptive constrained sparse quadrature to construct the surrogate model coefficients. Domain clustering methodologies are also employed to properly model plateaus and sharp discontinuities in the climate model observables.

Cosmin Safta, Khachik Sargsyan
Sandia National Laboratories
csafta@sandia.gov, ksargsy@sandia.gov

Daniel Ricciuto
Oak Ridge National Laboratory
ricciutodm@ornl.gov

Robert D. Berry
Sandia National Laboratories
rdberry@sandia.gov

Bert J. Debusschere
Energy Transportation Center
Sandia National Laboratories, Livermore CA
bjdebus@sandia.gov

Peter Thornton
Oak Ridge National Laboratory
thorntonpe@ornl.gov

Habib N. Najm
Sandia National Laboratories
Livermore, CA, USA
hnnajm@sandia.gov

MS59
Uncertainty in Regional Climate Experiments

climate models are subject to a number of different sources of uncertainty. Regional climate modeling introduce additional uncertainties associated with the boundary conditions and resolution of the models. In this talk, based on the ensemble being generated as part of the North American Regional Climate Assessment Program (NARCCAP), we will present statistical methodology for the analysis of the spatial-temporal output in the ensemble and quantifying the uncertainties associated with the NARCCAP experiment.

Stephan Sain
Institute for Mathematics Applied to Geosciences
National Center for Atmospheric Research
ssain@ucar.edu

MS60
Calibration, Model discrepancy and Extrapolative Predictions

In the presence of relevant physical observations, one can usually calibrate a computer model, and even estimate systematic discrepancies of the model from reality. Estimating and quantifying the uncertainty in this model discrepancy can lead to reliable predictions - so long as the prediction is "similar" to the available physical observations. Exactly how to define "similar" has proven difficult. Clearly it depends on how well the computational model captures the relevant physics in the system, as well as how portable the model discrepancy is, going from the available physical data to the prediction. This talk will discuss these concepts using computational models ranging from simple to very complex.

Dave Higdon
Los Alamos National Laboratory
Statistical Sciences

dhigdon@lanl.gov

MS60
Calibration, Validation and the Importance of Model Discrepancy

Extrapolation is inevitably accompanied by substantial uncertainty. To manage and quantify that uncertainty, calibration and validation are important tasks. But a fundamental feature underlying all these activities is model discrepancy, which is the difference between reality and the simulator output with "best" or "true" input values. This talk will show, both conceptually and through examples, that unless model discrepancy is acknowledged and carefully modeled calibration and extrapolations will be biased and over-confident.

Anthony O'Hagan
Univ. Sheffield, UK
a.ohagan@sheffield.ac.uk

Jenny Brynjarsdottir
Statistical and Applied Mathematical Sciences Institute
jenny.brynjarsdottir@gmail.com

MS60
"Experiment" and "Traveling" Models, Extrapolation Risk from Undetected Model Bias, and Data Conditioning for Systematic Uncertainty in Experiment Conditions

This talk will discuss some fundamental concepts and issues related to extrapolative prediction risk associated with model validation and conditioning. Topics will include: "traveling model" which travels to predictions beyond the validation or conditioning setting as a subset of the larger "experiment model" of the experiments; handling uncertainties accordingly; consistent and non-consistent bias and uncertainty in extrapolation; Type X validation or conditioning error from neglected systematic experimental uncertainty; data conditioning to mitigate associated prediction risk.

Vicente J. Romero
Validation and Uncertainty Quantification Department
Sandia National Laboratories
vjromer@sandia.gov

MS60
Towards Finding the Necessary Conditions for Justifying Extrapolations

A comprehensive approach is proposed to justify extrapolative predictions for models with known sources of error. The connection between model calibration, validation and prediction is made through the introduction of alternative uncertainty models used to model the localized errors. In addition a validation metric is introduced to provide a quantitative characterization of consistency of model predictions when compared with validation data. The talk will discuss the challenges in caring out the proposed methodology.

Gabriel A. Terejanu
Institute for Computational Engineering and Sciences
University of Texas at Austin
terejanu@ices.utexas.edu

Ernesto E. Prudencio
Institute for Computational Engineering and Sciences
prudenci@ices.utexas.edu

MS61
A Random Iterative Proper Orthogonal Decomposition Approach with Application to the Filtering of Distributed Parameter Systems

We consider the problem of filtering systems governed by partial differential equations. We propose a randomly perturbed iterative version of the snapshot proper orthogonal decomposition (POD) technique, termed RI-POD, to construct an ROM to capture the systems global behaviour. The technique is data based, and is applicable to forced as well as unforced systems. The ROM generated is used to construct reduced order Kalman filters to solve the filtering problem.

Suman Chakravorty
Texas A&M University
College Station, TX
schakrav@tamu.edu

MS61
A New Approach to Uq Based on the Joint Excitation-Response Pdf: Theory and Simulation

We study the evolution equation of joint excitation-response PDF obtained by Hopf functional approach for various stochastic systems. Some issues arising in this formulation are examined including, multiple available equations, representation of correlated random process, and etc. This approach is tested with Nonlinear Advection equation, Tumor cell model, Duffing Oscillator, and Limit Cycle Oscillator, and the results are compared.

Heyrim Cho
Brown University
Providence, RI
heyrim_cho@brown.edu

Daniele Venturi
Brown University
daniele_venturi@brown.edu

George E. Karniadakis
Brown University
Division of Applied Mathematics
george_karniadakis@brown.edu

MS61
Bayesian UQ on Infinite Dimensional Spaces with Incompletely Specified Priors

The Bayesian framework is popular way of handling data in UQ. This is done by defining priors on (possibly infinite dimensional) spaces of measures and functions and conditioning those priors after the observation of the sample data. It has been known since the earlier work of Diaconis and Freedman that, when the probability space allows for an infinite number of outcomes, the Bayesian posteriors, in general, do not converge towards the "true distribution.' In this work we compute optimal bounds on posteriors when priors in incompletely specified (through finite-dimensional marginals for instance). These bounds show that: (1) priors sharing the same finite dimensional marginals may lead to diverging posteriors under sample data (2) any desired

posterior can be achieved by a prior satisfying pre-specified finite-dimensional constraints (3) the measurement of sample data (in general) increases uncertainty instead of decreasing it if the classical Bayesian framework is applied ("as is') to an infinite (possibly high-dimensional) space. Finally, we develop a (OUQ) variant of the Bayesian framework that (1) allows to work with incompletely specified priors (2) remains consistent in infinite-dimensional spaces (whose posteriors converge towards the "true distribution') (3) provides optimal bounds on posteriors (4) leads to sharper estimates than those associated with the vanilla frequentist framework if the (incomplete) information on priors is accurate. This is a joint work with Clint Scovel (LANL) and Tim Sullivan (Caltech) and a sequel to an earlier work on Optimal Uncertainty Quantification (OUQ, http://arxiv.org/abs/1009.0679, joint with C. Scovel, T. Sullivan, M. McKerns (Caltech) and M. Ortiz (Caltech)).

Houman Owhadi
Applied Mathematics
Caltech
owhadi@caltech.edu

MS61
Conjugate Unscented Transformation – "Optimal Quadrature"

This talk will introduce a recently developed Conjugate Unscented Transformation (CUT) to compute multidimensional expectation integrals. An extension of popular unscented transformation will be presented to find a minimal number of quadrature points that is equivalent to the Gaussian quadrature rule of same order. Equivalent to same order implies that both the new reduced quadrature point set and the Gaussian quadrature product rule exactly reproduce the expectation integral involving a polynomial function of order d.

Nagavenkat Adurthi
MAE Deaprtment
University at Buffalo
n.adurthi@gmail.com

Puneet Singla
Mechanical & Aerospace Engineering
University at Buffalo
p.singla@gmail.com

Tarunraj Singh
Dept of Mechanical Engineering
SUNY at Buffalo
tsingh@buffalo.edu

MS62
Perspectives on Quantifying Uncertain Mechanisms in Dynamical Systems

Due to lack of scientific understanding, some mechanisms are not always well-represented in mathematical models for complex systems. The impact of these uncertain mechanisms on the overall system evolution may be delicate or even profound. These uncertain mechanisms are sometimes microscopic, and it is desirable to examine how they affect the system at the macroscopic level since we are often mainly interested in macroscopic dynamics. The speaker presents an overview of several available analytical and computational techniques for extracting macroscopic dynamics, while taking uncertain microscopic mechanisms into account. The issues include quantifying uncertain mechanisms via probability distributions, dynamical averaging of random slow-fast microscopic mechanisms, ensemble averaging of fluctuating driving forces, and especially, data-driven quantification of uncertain mechanisms in water vapor dynamics.

Jinqiao Duan
Institute for Pure and Applied Mathematics
UCLA
jduan@ipam.ucla.edu

MS62
Stochastic Integrable Dynamics of Optical Pulses Propagating through an Active Medium

Resonant interaction of light with a randomly-prepared, lambda-configuration active optical medium is described by exact solutions of a completely-integrable, stochastic partial differential equation, thus combining the opposing concepts of integrability and disorder. An optical pulse passing through such a material will switch randomly between left- and right-hand circular polarizations. Exact probability distributions of the electric-field envelope variables describing the light polarization and their switching times will be presented .

Gregor Kovacic
Rensselaer Polytechnic Inst
Dept of Mathematical Sciences
kovacg@rpi.edu

Ethan Atkins
Courant Institute
atkins@cims.nyu.edu

Peter R. Kramer
Rensselaer Polytechnic Institute
Department of Mathematical Sciences
kramep@rpi.edu

Ildar R. Gabitov
Department of Mathematics, University of Arizona
gabitov@math.arizona.edu

MS62
Reduced Models for Mode-locked Lasers with Noise

We explore the impact of spontaneous emissions noise on mode-locked laser linewidth by using a variational technique to reduce the original model, a stochastic partial differential equation, to a low-dimensional stochastic ordinary differential equation. The joint distribution of the parameters is mapped to a full-width half-maximum measure of the output laser linewidth, i.e., frequency uncertainty. Events causing the linewidth to exceed a prescribed uncertainty level are rare, requiring the application of large deviations theory or importance sampling approaches.

Richard O. Moore, Daniel S. Cargill
New Jersey Institute of Technology
rmoore@njit.edu, dc26@njit.edu

Tobias Schaefer
Department of Mathematics
The College of Staten Island, City University of New York
tobias@math.csi.cuny.edu

MS62
Analysis and Simulations of a Perturbed Stochastic Nonlinear Schrödinger Equation for Pulse Propagation in Broadband Optical Fiber Lines

We study the interplay between bit pattern randomness, Kerr nonlinearity, and delayed Raman response in broadband multichannel optical fiber transmission lines. We show that pulse propagation can be described by a perturbed stochastic nonlinear Schrödinger equation, which takes into account changes in pulse amplitude, group velocity, and position. Numerical simulations with the stochastic PDE along with analysis of the corresponding stochastic reduced ODE model are used to calculate the bit-error-rate and to identify the major error-generating processes in the fiber line.

Avner Peleg
State University of New York at Buffalo
apeleg@buffalo.edu

Yeojin Chung
Southern Methodist University
ychung@mail.smu.edu

MS63
Quantification of Uncertainty in Wind Energy

Abstract not available at time of publication.

Karthik Duraisamy
Stanford
dkarthik@stanford.edu

MS63
Uncertainty Quantification for Rayleigh-Taylor Turbulent Mixing

We present two main results. First: a reformulation of convergence for simulations of turbulent flow, through binning solution values from neighboring points (in a "supercell") to define a finite approximation to a space-time dependent probability density function. We thereby obtain convergence of fluctuations, and of nonlinear functions of the solution. Second: to reconstruct initial conditions (often not recorded) from early time data with uncertainty bounds on the reconstruction and on the entire solution.

Tulin Kaman
SUNY Stony Brook
tkaman@ams.sunysb.edu

James Glimm
State University of New York, Stony Brook
glimm@ams.sunysb.edu

MS63
Case Studies in Uncertainty Quantification for Aerodynamic Problems in Turbomachinery

In this study, we study the use of common UQ methods for problems of importance in practical engineering designs. In particular, we assess the efficiency of common polynomial chaos basis functions and sampling techniques like Smolyak-grids. The computational frame-work will be first validated against Monte-Carlo simulations to assess convergence of pdfs. It will then be used to assess the variability in compressor blade efficiency and turbine vane loss due to uncertainty in inflow conditions. The results will be used to answer the following questions: Do we need new probabilistic algorithms to quantify the impact of uncertainty? What is the optimal basis for standard performance metrics in turbomachinery? What are the computational and accuracy requirements of this probabilistic approach? Are there alternate (more efficient) techniques? We believe that the answers to the above questions will provide a quantitative basis to assess the usefulness of non-intrusive (and possibly intrusive) probabilistic methods to analyze variability in engineering designs.

Sriram Shankaran
General Electric
shankaran@ge.com

MS64
Prior Modelling for Inverse Problems Using Gaussian Markov Random Fields

In inverse problems, regularization functions are often chosen to incorporate prior information about a spatially distributed parameter, such as differentiability. In contrast, a standard Bayesian approach assumes that the value of each parameter is Gaussian with mean and variance dependent upon the values of its neighbors. This approach leads to a so-called Gaussian Markov random field prior. We will explore the interesting connections between these two approaches, which in many cases yield equivalent variational problems.

Johnathan M. Bardsley
University of Montana
bardsleyj@mso.umt.edu

MS64
Evaluation of Covariance Matrices and their use in Uncertainty Quantification

Abstract not available at time of publication.

Eldad Haber
Department of Mathematics
The University of British Columbia
haber@math.ubc.ca

MS64
Challenges in Uncertainty Quantification for Dynamic History Matching

The inversion of large scale ill-posed problems introduces multiple challenges. Examples would be: how to prescribe a suitable regularizer, design an informative experiment, quantify uncertainty, exploit supplementary information from multiple sources, or even how to define an appropriate optimization scheme. In the context of flow in porous medium, subsurface parameters are inferred through inversion of oil production data in a process called history matching. In this talk the inherent uncertainty of the problem is tackled in terms of prior sampling. Despite meticulous efforts to minimize the variability of the solution space, the distribution of the posterior may remain rather intrusive. In particular, geo-statisticians often propose large sets of prior samples that regardless of their apparent geological distinction are almost entirely flow equivalent. As an antidote, a reduced space hierarchical clustering of flow-relevant indicators is proposed for aggregation of these samples. The effectiveness of the method is demonstrated both with synthetic and real field data. This research was

performed as part of IBM-Shell joint research project.

Lior Horesh
Business Analytics and Mathematical Sciences
IBM TJ Watson Research Center
lhoresh@us.ibm.com

Andrew R. Conn
IBM T J Watson Research Ctr
arconn@us.ibm.com

Gijs van Essen, Eduardo Jimenez
Shell Innovation Research & Development
gijs.vanessen@shell.com, eduardo.jimenez@shell.com

Sippe Douma
Shell
sippe.douma@shell.com

Ulisses Mello
IBM Watson Research Center
ulissesm@us.ibm.com

MS64
Title Not Available at Time of Publication

Abstract not available at time of publication.

Luis Tenorio
Colorado School of Mines
ltenorio@mines.edu

MS65
The Influence of Topology on Sound Propagation in Granular Force Networks

Granular materials have been modelled using both continuum and particulate perspectives but neither approach can capture complex behaviours during sound propagation. A network representation provides an intermediate approach that allows one to directly consider microscopic features and longer-range interactions, e.g. force chains. In experiments on granular materials composed of photoelastic particles, we characterise the internal force structure and show that weighted meso-scale network diagnostics are crucial for quantifying sound propagation in this heterogeneous medium.

Danielle S. Bassett
University of California Santa Barbara
dbassett@physics.ucsb.edu

Eli Owens, Karen Daniels
North Carolina State University
etowens@ncsu.edu, kdaniel@ncsu.edu

Mason A. Porter
University of Oxford
Oxford Centre for Industrial and Applied Mathematics
porterm@maths.ox.ac.uk

MS65
Size of Synchronous Firing Events in Model Neuron Systems

We investigate the interaction of synchronous dynamics and the network topology in simple pulse-coupled Markov chain models for neuron dynamics. Theories for predicting the size of synchronous firing events are presented, in which the probabilistic dynamics between these events are taken into account. We use the theories to find different model networks that preserve the global dynamics on these networks.

Katherine Newhall
Rensselaer Polytechnic Institute
newhall@cims.nyu.edu

MS65
Network Analysis of Anisotropic Electrical Properties in Percolating Sheared Nanorod Dispersions

Percolation in nanorod dispersions induces extreme properties, with large variability near the percolation threshold. We investigate electrical properties across the dimensional percolation phase diagram of sheared nanorod dispersions [Zheng et al., Adv. Mater. 19, 4038 (2007)]. We quantify bulk average properties and corresponding fluctuations over Monte Carlo realizations, including finite size effects. We also identify fluctuations within realizations, with special attention on the tails of current distributions and other rare nanorod subsets which dominate the electrical response.

Feng B. Shi
UNC, Chapel Hill
bill10@live.unc.edu

Mark Forest
University of North Carolina at Chapel Hill
forest@amath.unc.edu

Peter J. Mucha
University of North Carolina
mucha@unc.edu

Simi Wang
University of North Carolina at Chapel Hill
wangsimi@email.unc.edu

Xiaoyu Zheng
Dept of Mathematics
Kent State University
zheng@math.kent.edu

Ruhai Zhou
Old Dominion University
ruhai@email.unc.edu

MS65
Asymptotically Inspired Moment-Closure Approximation for Adaptive Networks

Adaptive social networks, in which nodes and network structure co-evolve, are often described using a mean-field system of equations for the density of node and link types. These equations constitute an open system due to dependence on higher order topological structures. We propose a moment-closure approximation based on the analytical description of the system in an asymptotic regime. We show a good agreement between the improved mean-field prediction and simulations of the full network system.

Maxim S. Shkarayev
Mathematical Science Department, Rensselaer Polytech

Inst.
maxim.shkarayev@gmail.com

Leah Shaw
College of William and Mary
Dept. of Applied Science
lbshaw@wm.edu

MS66

Propagating Uncertainty from General Circulation Models through Projected Local Impacts

We develop statistical methodologies for impact analysis of climate change for economically important sectors, and transfer this development to the design of decision-support tools. Our approach is to implementin the context of specific regions and sensitive sectors of high economic and social importancetools that allow a coherent characterization of the propagation of uncertainty all the way to projected impacts, appropriately equipped with confidence or credibility statements relevant to the quantification of risks.

Peter Guttorp
University of Washington
peter@stat.washington.edu

MS66

Measures of Model Skill and Parametric Uncertainty Estimation for Climate Model Development

Measures of model skill and parametric uncertainty estimation for climate model development.

Gabriel Huerta
Indiana University
gahuerta@indiana.edu

Charles Jackson
UTIG
University of Texas at Austin
charles@ig.utexas.edu

MS66

Optimal Parameter Estimation in Community Atmosphere Models

The current tuning process of parameters in global climate models is often performed subjectively or treated as an optimization procedure to minimize model biases based on observations. In this study, a stochastic important-sampling algorithm, Multiple Very Fast Simulated Annealing (MVFSA) was employed to efficiently sample the input parameters in the KF scheme based on a skill score so that the algorithm progressively moved toward regions of the parameter space that minimize model errors.

Guang Lin, Ben Yang, Yun Qian, Ruby Leung
Pacific Northwest National Laboratory
guang.lin@pnnl.gov,   ben.yang@pnnl.gov,
yun.qian@pnnl.gov, ruby.leung@pnnl.gov

MS66

Covariance Approximation for Large Multivariate Spatial Datasets with An Application to Multiple Climate Models

In this work we investigate the cross-correlations across multiple climate model errors. We build a Bayesian hierarchical model that ac- counts for the spatial dependence of individual models as well as cross-covariances across different climate models. Our method allows for a non-separable and non-stationary cross-covariance structure. We also present a covariance approximation approach to facilitate the computation in the modeling and analysis of very large multivariate spatial data sets. The covariance approximation consists of two parts: a reduced-rank part to capture the large-scale spatial dependence, and a sparse covariance matrix to correct the small-scale dependence error induced by the reduced rank approximation. Simulation results of model fitting and prediction show substantial improvement of the proposed approximation over the predictive process approximation and the independent blocks analysis. We then apply our computational approach to the joint statistical modeling of multiple climate model errors.

Huiyan Sang
Texas A&M University
huiyan@stat.tamu.edu

MS67

Validation Experience for Stochastic Models of Groundwater Flow and Radionuclide Transport at Underground Nuclear Test Sites and the Shift Away from Quantitative Measures and Toward Iterative Improvement

Several groundwater models of underground nuclear tests, incorporating uncertainty, were subjected to validation processes. There were failures in balancing readily quantifiable and measurable model attributes against harder-to-measure conceptual issues, in gaining decision-maker acceptance of statistically based conclusions, and ultimately in the quality and quantity of data forming the foundation of the original models. From this experience, the regulatory framework has shifted away from validation and toward a model evaluation approach with an emphasis on iterative improvement.

Jenny Chapman
Desert Research Institute
jenny.chapman@dri.edu

Ahmed Hassan
Irrigation and Hydraulics Department
Cairo University
ahmed.hassan@dri.edu

Karl Pohlmann
Desert Research Institute
karl.pohlmann@dri.edu

MS67

Validation and Data Assimilation of Shallow Water Models

We will discuss the validation of large-scale coupled wave-current models for simulating hurricane storm surge. We will demonstrate that by including the appropriate physics, discretizations, and parameters, one can consistently match measured data from a wide range of hurricanes. However, we will also point out where the models have significant uncertainty and describe a new data-assimilation framework for real-time hurricane surge forecasts.

Clint Dawson

Institute for Computational Engineering and Sciences
University of Texas at Austin
clint@ices.utexas.edu

Jennifer Proft, J. Casey Dietrich
University of Texas at Austin
jennifer@ices.utexas.edu, dietrich@ices.utexas.edu

Troy Butler
Institute for Computational Engineering and Sciences
University of Texas at Austin
tbutler@ices.utexas.edu

Talea Mayo
University of Texas at Austin
talea@ices.utexas.edu

Joannes Westerink
Department of Civil Engineering and Geological Sciences
University of Notre Dame
jjw@nd.edu

Ibrahim Hoteit
King Abdullah University of Science and Technology
(KAUST)
ibrahim.hoteit@kaust.edu.sa

M.U. Altaf
King Abdullah University of Science and Technology
m.u.altaf@ewi.tudelft.nl

MS67

Quantifying Long-Range Predictability and Model Error through Data Clustering and Information Theory

We present a framework blending data clustering and information theory to quantify long-range initial-value predictability and forecast error with imperfect models in complex dynamical systems. With reference to wind-driven ocean circulation, we demonstrate that the pertinent information for long-range forecasting can be represented via a coarse-grained partition of the set of initial data available to a model. A related formalism is applied to assess the forecast skill of Markov models of ocean circulation regimes.

Dimitris Giannakis
New York University
dimitris@cims.nyu.edu

MS67

Model Selection and Inference for a Nuclear Reactor Application

We compare statistical techniques for model selection, with a focus on information theoretic approaches, applied in a statistical framework for calibration of computer codes. Additionally, we propose a sequential strategy for iterative refinement of importance distributions used to sample uncertain model inputs to estimate the probability that a calibrated model exceeds a fixed or random threshold. We demonstrate these methods on a nuclear reactor application involving calculation of peak coolant temperature with the R7 code.

Laura Swiler
Sandia National Laboratories

Albuquerque, New Mexico 87185
lpswile@sandia.gov

Brian Williams, Rick Picard
Los Alamos National Laboratory
brianw@lanl.gov, picard@lanl.gov

MS68

Uncertainty Quantification and Model Validation in Flight Control Applications

Models derived from physics or data are often too complicated for analysis or controller design. This is leads to reduced order modeling. However, it is important to assess the quality of such models. Often, for nonlinear systems in particular, model validation is performed using Monte-Carlo simulations. Two systems are qualified to be similar if the variance of the trajectories are small. In this paper, we present a new paradigm where two systems are qualified to be similar if the density function of the output is similar, when excited by the same random input. This is more general than comparing few moments or the support of the trajectories. We use Wasserstein distance to compare density functions and also argue why the commonly use Kullback-Liebler metric is unsuitable for model validation. Examples based on flight control problems are presented to illustrate model validation in this framework.

Raktim Bhattacharya
Texas A&M University
College Station, Texas
raktim@tamu.edu

MS68

New Positive-definite Random Matrix Ensembles for Stochastic Dynamical System with High Level of Heterogeneous Uncertainties

The scientific community has seen an increasing surge of applications of positive-definite random matrix ensembles in the fields of mechanics and multiscale mechanics in recent years. These ensembles are employed to *directly* model several positive-definite matrix-valued objects, e.g., mass matrices, stiffness matrices, constitutive elasto-plasticity tensor, etc. Matrix variate distributions, e.g., Wishart/Gamma distribution, Beta Type 1 distribution, Kummer-Beta distribution, or distributions derived from them, are currently considered for this modeling purpose. These distributions are, however, parameterized such that they induce specific mean and covariance structures that do not allow sufficient flexibility in modeling high level of uncertainties. The current work will discuss two new positive-definite random matrix ensembles that are likely to provide more flexibility in modeling high level of uncertainties.

Sonjoy Das, Sonjoy Das
University at Buffalo
sonjoy@buffalo.edu, sonjoy@buffalo.edu

MS68

Existence and Stability of Equilibria in Stochastic Galerkin Methods

We consider dynamical systems in form of nonlinear autonomous ordinary differential equations including random parameters. Thus the corresponding solutions represent random processes. The existence of a unique stable equi-

librium is assumed for each sample of the parameters. Thereby, the equilibria depend on the random parameters. We apply the polynomial chaos expansion of the unknown random process to solve the stochastic dynamical system. The stochastic Galerkin method yields a larger coupled system of nonlinear ordinary differential equations satisfied by an approximation of the random process. The existence of equilibria is investigated for the coupled system. Moreover, we analyze the stability of these fixed points, where the spectrum of a Jacobian matrix has to be examined. Numerical simulations of test examples are presented.

Roland Pulch
University of Wuppertal
pulch@math.uni-wuppertal.de

MS68
A Nonlinear Dimension Reduction Technique for Random Fields Based on Topology-Preserving Transformations

The intrinsic dimensionality of a random field may be defined as the minimum number of degrees of freedom which is neccessary to account for its relevant statistical information. In this talk we will present a new nonlinear dimension reduction technique for random fields based on latent variable models and topology-preserving transformations. The low-dimensional embedding will be explicitly constructed together with the probability measure associated with the reduced-order probability space.

Daniele Venturi
Brown University
daniele_venturi@brown.edu

Guang Lin
Pacific Northwest National Laboratory
guang.lin@pnnl.gov

George E. Karniadakis
Brown University
Division of Applied Mathematics
george_karniadakis@brown.edu

MS69
New Results for the Stochastic PDEs of Fluid Dynamics

The addition of white noise driven terms to the fundamental equations of physics and engineering are used to model numerical and empirical uncertainties. In this talk we will discuss some recent results for the Stochastic Navier-Stokes and Euler Equations as well as for the Stochastic Primitive Equations, a basic model in geophysical scale fluid flows. For all of the above systems our results cover the case of a general nonlinear multiplicative stochastic forcing.

Nathan Glatt-Holtz
Indiana University
negh@indiana.edu

MS69
Asymptotic Behavior of Stochastic Lattice Differential Equations

Random attractor is an important concept to describe long-term behavior of solutions for a given stochastic system. In this talk we will first provide sufficient conditions for the existence of a global compact random attractors for general dynamical systems in weighted space of infinite sequences. We then apply the result to show the existence of a unique global compact random attractor for first order, second order and partly dissipative stochastic lattice differential equations with random coupled coefficients and multiplicative/additive white noise in weighted spaces.

Xiaoying Han
Auburn University
xzh0003@auburn.edu

MS69
Unbiased Perturbations of the Navier-Stokes Equation

We consider a new class of stochastic perturbations of the Navier-Stokes equation. Its unique feature is the preservation of the mean dynamics of the deterministic equation, hence it is an unbiased random perturbation of the equation. We will discuss results for the steady state solutions and the convergence to steady solutions, and show sufficient conditions which are very similar to analogous results for the unperturbed equation. Numerical simulations comparing this unbiased perturbation with the usual stochastic Navier-Stokes will be shown.

Chia Ying Lee
Statistical and Applied Mathematical Sciences Institute
U. of North Carolina
cylee@samsi.info

Boris Rozovsky
Brown University
rozovsky@dam.brown.edu

MS69
Generalized Malliavin Calculus and Spdes in Higher-Order Chaos Spaces

The Malliavin derivative, divergence operator (Skorokhod integral), and the Ornstein-Uhlenbeck operator are extended from the traditional Gaussian setting, or first-order chaos space, to nonlinear generalized functionals of white noise, which are elements of the full chaos space. These extensions are then applied to study stochastic elliptic and parabolic equations driven by noise from higher-order chaos spaces.

Sergey Lototsky
Department of Mathematics
University of Southern California
lototsky@usc.edu

Boris Rozovskii
Brown University
boris_rozovsky@brown.edu

Dora Selesi
University of Novi Sad
dora.selesi@dmi.uns.ac.rs

MS69
Stochastic-Integral Models for Propagation-of-Uncertainty Problems in Nondestructive Evaluation

Generalized polynomical chaos (gPC) and the probabilistic

collocation method (PCM) are finding considerable application to problems of interest to engineers in which random parame- ters are an essential feature of the mathematical model. So far the applications have been mainly to stochastic partial differential equations, but we extend the method to volume-integral equations, which have met great success in electromagnetic nondestructive evaluation (NDE), especially with eddy-currents. The problems of main interest to the NDE community in this connection are concerned with the issue of propagation of uncertainty when the relevant parameters are not well characterized, or are known simply as random variables. We demonstrate the ideas by considering a metallic surface that has undergone a shot-peening treatment to reduce residual stresses, and has, therefore, become a random conductivity field.

Elias Sabbagh
Victor Technologies
ehs@sabbagh.com

Kim Murphy, Harold Sabbagh
Victor Technologies, LLC
kimmurphy1@aristotle.net, has@sabbagh.com

John Aldrin
Computationaltools
aldrin@computationaltools.com

Jeremy Knopp
Air Force Research Laboratory
Jeremy.Knopp@wpafb.af.mil

Mark Blodgett
Air Forch Research Laboratory
mark.blodgett@wpafb.af.mil

MS70
Hybrid Methods for Data Assimilation

I present a theoretical comparison of two widely used data assimilation methods: the ensemble Kalman filter (EnKF) approach and the four dimensional variational (4D-Var) approach. Then I propose a suboptimal hybridization scheme to combine the advantages of the EnKF and the 4D-Var. This new hybrid technique is computationally less expensive than the full 4D-Var and, in simulations, performs better than EnKF for both linear and nonlinear test problems.

Haiyan Cheng
Willamette University
hcheng@willamette.edu

Adrian Sandu
Virginia Polytechnic Institute and
State University
sandu@cs.vt.edu

MS70
Model Covariance Sensitivity as a Guidance for Localization in Data Assimilation

In this talk we present how to use model covariance sensitivity information to guide, in a more precise manner, the selection of appropriate cross-correlation length-scale parameters for model covariance localization techniques. Covariance sensitivities are obtained using adjoint-based methods. Numerical experiments are presented for the ensemble Kalman filter data assimilation applied to the Lorenz 40-variable model. The relevance of the technique, as well as its utility, for operational data assimilation systems will be presented and discussed.

Humberto C. Godinez
Los Alamos National Laboratory
Applied Mathematics and Plasma Physics
hgodinez@lanl.gov

Dacian N. Daescu
Portland State University
Department of Mathematics and Statistics
daescu@pdx.edu

MS70
The Estimation of Functional Uncertainty using Polynomial Chaos and Adjoint Equations

The combined use of nonintrusive polynomial chaos (PC) and adjoint equations (yielding the gradient) is addressed aimed at the estimation of uncertainty of a valuable functional subject to large errors in the input data. Random variables providing maximum impact on the result (leading values) may be found using the gradient information that allows reduction of the problem dimension. The gradient may be also used for the calculation of PC coefficients, thus enabling further acceleration of the computations. Using gradient information for the estimation of polynomial coefficients (APC) also provides a significant reduction of the computation time. The adjoint Monte VCarlo (AMC)is highly efficient from a computational viewpoint and accurate for moderate amplitude of errors. For a large number of random variables, the accuracy of AMC is close (or even superior) to PC results even under large error.

Michael Navon
Florida State University
inavon@fsu.edu

MS70
FATODE: A Library for Forward, Tangent Linear, and Adjoint ODE Integration

FATODE is a FORTRAN library for the integration of ordinary differential equations with direct and adjoint sensitivity analysis capabilities. The paper describes the capabilities, implementation, code organization, and usage of this package. FATODE implements the forward, adjoint, and tangent linear models for four families of methods — ERK, FIRK, SDIRK, and Rosenbrock. A wide range of applications are expected to benefit from its use; examples include parameter estimation, data assimilation, optimal control, and uncertainty quantification.

Hong Zhang
Virginia Tech
zhang@vt.edu

Adrian Sandu
Virginia Polytechnic Institute and
State University
sandu@cs.vt.edu

MS71
Upscaling
Micro-scale Material Variability Through the use

of Random Voronoi Tessellations

A randomly seeded Voronoi tessellation is used to model the microscale grain structure of a thin ductile ring. Each grain is assigned an elastic stiffness tensor with cubic symmetry but with randomly oriented principal directions. The ring is subjected to internal pressure loading and deformed elastically. The displacement and stress response of the ring is studied from the perspective of homogenization theory as the ratio of the grain size to ring diameter is varied.

Joseph Bishop
Sandia National Laboratory
jebisho@sandia.gov

MS71
Discrete Models of Fracture and Mass Transport in Cement-based Composites

The life-cycle performance of structural concrete is affected by material features and internal processes that span several length scales. This presentation regards the discrete lattice modeling of such features, fracture, and crack-assisted mass transport in concrete. Domain discretization is based on Voronoi/Delaunay tessellations of semi-random point sets. Lack of scale separation complicates the modeling efforts. Variability is quantified by simulating multiple, random realizations of nominally identical structures.

John Bolander
UC Davis
jebolander@ucdavis.edu

Peter Grassl
School of Engineering
University of Glasgow
peter.grassl@glasgow.ac.uk

MS71
Maximal Poisson-disk Sampling for UQ Purposes

We describe a new approach to solve the maximal Poisson-disk sampling in d-dimensional spaces for UQ purposes. In contrast to existing methods, our technique tracks the remaining voids after a classical dart throwing phase by constructing the associated convex hulls. This provides a mechanism for termination with bounded time complexity. We also show how to utilize this sampling techniques to achieve better estimations of probability of failure and detection of discontinuities. We demonstrate application examples.

Mohamed S. Ebeida
Sandia National Laboratories
msebeid@sandia.gov

MS71
Simplex Stochastic Collocation Approach

The Simplex Stochastic Collocation method is introduced as an non-intrusive, adaptive un- certainty quantification method for computational problems with random inputs. The effectiveness of adaptive formulation is determined by both h- and p-refinement measures and a stopping criterion derived from an error estimate based on hierarchical surpluses. A p-criterion for the polynomial degree p is formulated to achieves a constant order of convergence with dimensionality. Numerical results show that the stopping criterion is reliable owing to the accurate and conservative error estimate, and that the refinement measures outperform uniform refinement.

Gianluca Iaccarino
Stanford University
jops@stanford.edu

Jeroen Witteveen
Stanford University
Center for Turbulence Research
jasw@stanford.edu

MS71
Random Poisson-Disk Samples and Meshes

Maximal Poisson-disk sampling produces random point clouds of uniform density. Every part of the domain is within distance r of a sample, yet no two samples are closer than r to each other. I will describe an optimal algorithm for generating samples, and how we sample the domain boundary differently to get a Delaunay triangle or Voronoi polyhedral mesh. These meshes have provable quality similar to determinist meshes, but with uniform random orientations.

Scott A. Mitchell, Mohamed S. Ebeida
Sandia National Laboratories
samitch@sandia.gov, msebeid@sandia.gov

MS72
Quantile Emulation for Non-Gaussian Stochastic Models

Stochastic models often require a large number of expensive runs for practical applications. In the emulator framework, the model is replaced with a faster surrogate (a Gaussian process) which captures prediction uncertainty under the assumption of Gaussianity. If the simulator response is non-Gaussian however, alternative approaches have to be sought. We investigate emulation of quantiles and discuss how to perform Bayesian inference for this class of models. A real world example application is provided.

Remi Barillec
University of Aston, UK
Non-linearity and Complexity Research Group
r.barillec@aston.ac.uk

Alexis Boukouvalas, Dan Cornford
University of Aston, UK
boukouva@aston.ac.uk, d.cornford@aston.ac.uk

MS72
Methods for Assessing Chances of Rare, High-Consequence Events in Groundwater Monitoring

This talk looks at multiple approaches for assessing uncertainty in high-consequence, low probability events related to groundwater monitoring. We consider Monte Carlo, Markov chain Monte Carlo, and null-space Monte Carlo, all of which have difficulty estimating the chance of low probability events. We also look at modifications to these approaches that help address this issue. We focus on a synthetic application in 3d solute transport.

Dave Higdon
Los Alamos National Laboratory

Statistical Sciences
dhigdon@lanl.gov

Elizabeth Keating, Zhenxue Dai, James Gattiker
Los Alamos National Laboratory
ekeating@lanl.gov, daiz@lanl.gov, gatt@lanl.gov

MS72
Sensitivity Analysis and Estimation of Extreme Tail Behaviour in Two-dimensional Monte Carlo Simulation (2DMC)

Two-dimensional Monte Carlo simulation is frequently used to implement risk models, comprising mechanistic and probabilistic components, to separately quantify uncertainty and variability within a population. Risk managers must assess the proportion exceeding a critical threshold, and the levels of exceedence. We describe an efficient method combining Bayesian model emulation and extreme value theory, which can also be used to quickly identify those model parameters having the greatest impact on the probabilities of rare events.

Marc C. Kennedy, Victoria Roelofs
The Food and Environment Research Agency
marc.kennedy@fera.gsi.gov.uk,
victoria.roelofs@fera.gsi.gov.uk

MS72
An Investigation of the Pineapple Express Phenomenon via Bivariate Extreme Value Theory

We apply bivariate extreme value methods in an examination of extreme winter precipitation events produced by a regional climate model. We first assess the model's ability to reproduce these events in the US Pacific coast region. We then link these events to large-scale process dynamics, with a particular focus on the pineapple express (PE), a special type of winter event. Finally, we examine extreme events produced by the model in a future climate scenario.

Grant Weller
Department of Statistics,
Colorado State University
weller@stat.colostate.edu

Dan Cooley
Colorado State University
cooleyd@stat.colostate.edu

Stephan Sain
Institute for Mathematics Applied to Geosciences
National Center for Atmospheric Research
ssain@ucar.edu

MS73
An Introduction to Emulators and Climate Models

State of the art climate simulators pose particular problems for UQ methods. They have very large state spaces ($o10^{12}$) and are computationally expensive. In this talk I will introduce climate models, what they do, how they work and the problems that arise when we quantify their uncertainty, identify its source and use data to reduce it. I will outline some solutions to these , where the current challenges lie and outline future research.

Peter Challenor
National Oceanography Centre, Southampton, UK
p.challenor@noc.ac.uk

MS73
Calibration of Gravity Waves in WACCM

The Whole Atmosphere Community Climate Model (WACCM) is a comprehensive numerical model, spanning the range of altitude from the Earth's surface to the thermosphere. Gravity waves are a key component of the dynamics, and are parametrized. However, the current parametrization does not result in fully realistic features such as the period of the quasi-biennial oscillation. We carry out a Bayesian calibration of the gravity waves scheme using efficient sequential design of experiments.

Serge Guillas
University College London
serge@stats.ucl.ac.uk

Hanli Liu
NCAR
liuh@ucar.edu

MS73
Uncertainty in Modeled Upper Ocean Heat Content Change using a Large Ensemble

We evaluate the uncertainty in the heat content change (ΔQ) in the top 700 meters in the ocean component of the CCSM3.0 model using an emulator created from a large member ensemble. A large ensemble of the CCSM3.0 ocean/ice system at a 3 degree resolution was created by varying parameters related to ocean mixing and advection. The outcomes are compared to four estimates using observational data. We explore how other modeled estimates of ΔQ from the CMIP3 ensemble can be understood in the context of this large ensemble.

Robin Tokmakian
Naval Postgraduate School
rtt@nps.edu

MS73
Emulating Time Series Output of Climate Models

The RAPIT project is concerned with the risk, probability and impacts of future changes to the Atlantic Meridional Overturning Circulation (AMOC) under anthropogenic forcing. Our principle resource is an unprecedented perturbed parameter ensemble, (order 10,000 runs), of the fully coupled, un-flux-adjusted climate model, HadCM3. We present dynamic methods for emulating the AMOC time series output by the model and explore the use of these emulators in helping to constrain future AMOC projections using different data sources and ocean monitoring systems.

Danny Williamson
Durham University
daniel.williamson@durham.ac.uk

MS74
A Non-intrusive Alternative to a Computational

Measure Theoretic Inverse

We develop a non-intrusive technique for extending the computational measure-theoretic methodology to problems where it is either infeasible or impractical to obtain derivative information from the map. We discuss various sources of errors in the methodology and how to address these.

Troy Butler
Institute for Computational Engineering and Sciences
University of Texas at Austin
tbutler@ices.utexas.edu

MS74
Inverse Function-based Methodology for UQ

There is a growing need of statistical methodology for problems addressing inverse sensitivity analysis in which there are one or multiple quantities of interest connected to the input space through a system of partial differential equations. Though Bayesian methodology has become quite popular in this setting, we explore potential non-Bayesian solutions using some newer ideas related to inverse function-based inference. The goal is to understand the distribution on the parameter space without use of priors.

Jessi Cisewski
Department of Statistics and Operations Research
University of North Carolina at Chapel Hill
cisewski@email.unc.edu

MS74
A Computational Approach for Inverse Sensitivity Problems using Set-valued Inverses and Measure Theory

We discuss a numerical method for inverse sensitivity analysis of a deterministic map from a set of parameters to a randomly perturbed quantity of interest. The solution method has two stages: (1) approximate the unique set-valued solution to the inverse problem and (2) apply measure theory to compute the approximate probability measure on the parameter space that solves the inverse problem. We discuss convergence and analysis of the method.

Donald Estep
Colorado State University
estep@math.colostate.edu or don.estep@gmail.com

MS74
Inverse Problem and Fisher's View of Statistical Inference

R. A. Fisher's fiducial inference has been the subject of many discussions and controversies ever since he introduced the idea during the 1930's. The idea experienced a bumpy ride, to say the least, during its early years and one can safely say that it eventually fell into disfavor among mainstream statisticians. However, it appears to have made a resurgence recently under various guises. For example under the new name generalized inference fiducial inference has proved to be a useful tool for deriving statistical procedures for problems where frequentist methods with good properties were previously unavailable. Therefore we believe that the fiducial argument of R.A. Fisher deserves a fresh look from a new angle. In this talk we first generalize Fisher's fiducial argument and obtain a fiducial recipe applicable in virtually any situation. We demonstrate this fiducial recipe on examples of varying complexity. We also investigate, by simulation and by theoretical considerations, some properties of the statistical procedures derived by the fiducial recipe showing they often posses good repeated sampling, frequentist properties. As an example we apply the recipe to interval observed mixed linear model. Portions of this talk are based on a joined work with Hari Iyer, Thomas C.M. Lee and Jessi Cisewski

Jan Hannig
Department of Statistics, University of North Carolina
jan.hannig@mac.com

MS75
Variable Selection and Sensitivity Analysis via Dynamic Trees with an application to Computer Code Performance Tuning

We introduce a new response surface methodology, dynamic trees, with an application to variable selection and an input sensitivity analysis. These methods are used to analyze automatic computer code tuning that combines classification and regression elements on large data sets. The talk will also highlight an R package implementing the methods, called dynaTree, which is available on CRAN.

Robert Gramacy
University of Chicago
rbgramacy@chicagobooth.edu

MS75
Bayesian Filtering in Large-Scale Geophysical Systems and Uncertainty Quantification

Bayesian filters compute the probability distribution of the system, thus readily provide a framework for uncertainty quantification and reduction. In geophysical applications, filtering techniques are designed to produce a small sample of state estimates, as a way to reduce computational burden. This, coupled with poorly known model-observation deficiencies, would lead to distribution estimates that are far from optimal, yet still provide meaningful estimates. We present this problem and discuss possible approaches to produce improved uncertainty estimates.

Ibrahim Hoteit
King Abdullah University of Science and Technology (KAUST)
ibrahim.hoteit@kaust.edu.sa

Bruce Cornuelle
University of California, San Diego
bcornuelle@ucsd.edu

Aneesh Subramanian
University of California, San Diego, USA
acsubram@ucsd.edu

Hajoon Song
University of California, Santa Cruz, USA
j0song@ucsd.edu

Xiaodong Luo
1King Abdullah University of Science and Technology (KAUST),
xiaodong.luo@nullkaust.edu.sa

MS75
On Data Partitioning for Model Validation

Validation processes usually require that experimental data be split into calibration and validation datasets. As this choice is often subjective, we introduce an approach based on the concept of cross-validation. The proposed method allows one to systematically determine the optimal partition and to address fundamental issues in validation, namely that the model 1) be evaluated with respect to the data and to predictions of quantities of interest; 2) be highly challenged by the validation set.

Rebecca Morrison
UT Austin
rebeccae.morrison@gmail.com

Corey Bryant
The University of Texas at Austin
Institute for Computational Engineering and Sciences
cbryant@ices.utexas.edu

Gabriel A. Terejanu
Institute for Computational Engineering and Sciences
University of Texas at Austin
terejanu@ices.utexas.edu

Serge Prudhomme
ICES
The University of Texas at Austin
serge@ices.utexas.edu

Kenji Miki
Institute for Computational Engineering and Sciences
University of Texas at Austin
kenji@ices.utexas.edu

MS75
Validation of a Random Matrix Model for Mesoscale Elastic Description of Materials with Microstructures

We present validation of a bounded random matrix model defining the constitutive elastic behavior of heterogeneous material. Using an experimental database of microstructures, we first construct a surrogate model in order to further the data, required for calibration and validation. We then recall the construction of the random matrix model characterizing the mesoscale apparent elasticity tensor of the material. Finally a procedure is presented to validate the model using observations resulting from fine scale simulations.

Arash Noshadravan
University of Southern California
noshadra@usc.edu

Roger Ghanem
University of Southern California
Aerospace and Mechanical Engineering and Civil Engineering
ghanem@usc.edu

Johann Guilleminot
Laboratoire de Modelisation et Simulation Multi Echelle
Universite Paris-Est
johann.guilleminot@univ-paris-est.fr

Ikshwaku Atodaria, Pedro Peralta
School for Engineering of Matter
Arizona State University
ikshwaku.atodaria@asu.edu, pperalta@asu.edu

MS76
Toward Analysis of Uncertainty in Chaotic Systems

Due to the exponential growth of small disturbances, uncertainty analysis in chaotic systems is challenging. For example, even for mean quantities, sensitivity analysis using a standard adjoint-based approach fails because the adjoint variables diverge. In this talk, recent work on uncertainty quantification for chaotic systems is described. In particular, several methods, including polynomial chaos expansions, are evaluated for capturing uncertainty in mean quantities using the Lorenz equations as a model problem.

Eleanor Deram
University of Texas at Austin
nora.deram@gmail.com

Todd Oliver
PECOS/ICES, The University of Texas at Austin
oliver@ices.utexas.edu

Robert D. Moser
University of Texas at Austin
rmoser@ices.utexas.edu

MS76
A Dynamically Weighted Particle Filter for Sea Surface Temperature Modeling

The sea surface temperature (SST) is an important factor of the earth climate system. We analyze the SST data of Caribbean Islands area after a hurricane using the radial basis function network-based dynamic model. Comparing to the traditional grid-based approach, our approach requires much less CPU time and makes the real-time forecast of SST doable on a personal computer.

Faming Liang
Texas A&M University
College Station, Texas
fliang@stat.tamu.edu

Duchwan Ryu
Department of Biostatistics
Medical College of Georgia
dryu@mcg.edu

Bani Mallick
Department of Statistics
Texas A&M University
bmallick@stat.tamu.edu

MS76
Characterization of the Effect of Uncertainty in Terrain Representations for Modeling Geophysical Mass Flows

In modeling flow on natural terrains a persistent and difficult problem is the effect of errors and uncertainties in the representation of the terrain. In this talk we will discuss the effect of such uncertainty on outputs from a geophysical mass flow model. We will then introduce methodology to systematically account for these uncertainties by using a model of the error and sampling it to create ensembles

of possible elevations.

Ramona Stefanescu
University at Buffalo
ers32@buffalo.edu

Abani K. Patra
SUNY at Buffalo
Dept of Mechanical Engineering
abani@eng.buffalo.edu

Marcus Bursik
Dept. of Geology
SUNY at Buffalo
mib@buffalo.edu

MS77
Statistical Inference Problems for Nonlinear SPDEs

We consider a parameter estimation problem to determine the drift coefficient for a large class of parabolci Stochastic PDEs driven by additive or multiplicative noise. We derive several different classes of estimators based on the first N Fourier modes of a sample path observed continuously on a finite time interval. We study the consistency and asymptotic normality of these estimators as number of Fourier coefficients increases, and we present some numerical simulation results.

Igor Cialenco
Illinois Institute of Technology
igor@math.iit.edu

MS77
Filtering the Navier Stokes Equations

Data assimilation refers to methodologies for the incorporation of noisy observations of a physical system into an underlying model in order to infer the properties of the state of the system (possibly including parameters). The model itself is typically subject to uncertainties, in the input data and in the physical laws themselves. This leads naturally to a Bayesian formulation in which the posterior probability distribution of the system state, given the observations, plays a central conceptual role. The aim of this paper is to use this Bayesian posterior probability distribution as a gold standard against which to evaluate various commonly used data assimilation algorithms. We study the 2D Navier-Stokes equations in a periodic geometry and evaluate a variety of sequential filtering approximations based on 3DVAR and on extended and ensemble Kalman filters. The performance of these data assimilation algorithms is quantified by comparing the relative error in reproducing moments of the posterior probability distribution. The primary conclusions of the study are that: (i) with appropriate parameter choices, approximate filters can perform well in reproducing the mean of the desired probability distribution; (ii) however these filters typically perform poorly when attempting to reproduce information about covariance; (iii) this poor performance is compounded by the need to modify the filters, and their covariance in particular, in order to induce filter stability and avoid divergence. Thus, whilst filters can be a useful tool in predicting mean behaviour, they should be viewed with caution as predictors of uncertainty. We complement this study with (iv) a theoretical analysis of the ability of the filters to estimate the mean state accurately, and we derive a non-autonomous

(S)PDE for this estimate in the continuous-time limit.

Kody Law
Mathematics Institute
University of Warwick
kodylaw@gmail.com

MS77
Adaptive Construction of Surrogates for Bayesian Inference

Surrogate models are often used to accelerate Bayesian inference in statistical inverse problems. Yet the construction of globally accurate surrogates for complex models can be prohibitive and in a sense unnecessary, as the posterior distribution typically concentrates on a small fraction of the prior support. We present a new adaptive approach that uses stochastic optimization (the cross-entropy method) to construct surrogates that are accurate over the support of the posterior distribution. Efficiency and accuracy are demonstrated via parameter inference in nonlinear PDEs.

Jinglai Li, Youssef M. Marzouk
Massachusetts Institute of Technology
jinglai@mit.edu, ymarz@mit.edu

MS77
Reimagining Diffusion Monte Carlo for Quantum Monte Carlo, Sequential Importance Sampling, Rare Event Simulation and More

Diffusion Monte Carlo was developed forty years ago within the Quantum Monte Carlo community to compute ground state energies of the Schrodinger operator. Since then the basic birth/death strategy of DMC has found its way into a wide variety of application areas. For example efficient resampling strategies used in sequential importance sampling algorithms (e.g. particle filters) are based on DMC. As I will demonstrate, some tempting generalizations of the basic DMC framework lead to an instability in the time discretization parameter. This instability has important consequences in, for example, applications of DMC in sequential importance sampling and rare event simulation. We suggest a modification of the basic DMC algorithm that eliminates this instability. In fact, the new algorithm is more efficient than DMC under any condition (parameter regime). We prove this as well as show numerically and analytically that it is stable in unstable regimes for DMC.

Jonathan Weare
University of Chicago
Department of Mathematics
weare@math.uchicago.edu

Martin Hairer
The University of Warwick
M.Hairer@Warwick.ac.uk

MS78
Computing and Using Observation Impact in 4D-Var Data Assimilation

Data assimilation combines information from an imperfect model, sparse and noisy observations, and error statistics, to produce a best estimate of the state of a physical system. Different observational data points have different contributions to reducing the uncertainty with which the state is estimated. In this paper we present a computational ap-

proach to quantify the observation impact for analyzing the effectiveness of the assimilation system, for data pruning, and for designing future sensor networks.

Alexandru Cioaca
Virginia Tech
alexgc@vt.edu

Adrian Sandu
Virginia Polytechnic Institute and
State University
sandu@cs.vt.edu

MS78
Error Covariance Sensitivity and Impact Estimation with Adjoint 4D-Var

The adjoint-data assimilation system (DAS) is presented as a feasible approach to evaluate the forecast sensitivity with respect to the specification of the observation and background error covariances in a four-dimensional variational DAS. A synergistic link is established between various techniques to analyze the DAS performance: observation sensitivity, error covariance sensitivity and impact estimation, and a posteriori diagnosis. Applications to atmospheric modeling and the current status of implementation at numerical weather prediction centers are discussed.

Dacian N. Daescu
Portland State University
Department of Mathematics and Statistics
daescu@pdx.edu

MS78
Lagrangian Data Assimilation

Abstract not available at time of publication.

Christopher Jones
University of North Carolina and University of Warwick
ckrtj@email.unc.edu

MS78
Uncertainty Quantification and Data Assimilation Issues for Macro-Fiber Composite Actuators

Macro-fiber composites (MFC) are being considered for a range of present and emerging applications, such as flow control and remote configuration of large space structures, due to their large bandwidth, moderate power requirements, and moderate stain capabilities. However, they also exhibit hysteresis and constitutive nonlinearities due to their PZT components. In this presentation, we will discuss uncertainty quantification and data assimilation techniques for these actuators within the context of the homogenized energy modeling framework. This will utilize data collected under a variety of operating regimes.

Ralph C. Smith
North Carolina State Univ
Dept of Mathematics, CRSC
rsmith@eos.ncsu.edu

Zhengzheng Hu
Department of Mathematics
North carolina State University
zhu4@ncsu.edu

Nathanial Burch
SAMSI
nathanial.burch@gmail.com

MS79
Analyzing Predictive Uncertainty using Paired Complex and Simple Models

In analyzing the uncertainty of environmental model predictions a tension exists between the prior information and likelihood terms of Bayes Equation. The first requires a complex model that reflects the complexity of earth processes. The second requires a simple, fast-running model that can capture information from historical data. Use of a single model to achieve both erodes its ability to achieve either. A paired model approach can achieve the same ends with fewer compromises.

John Doherty
Flinders University and
Watermark Numerical Computing
johndoherty@ozemail.com.au

MS79
Modeling Spatial Variability as Measurement Uncertainty

Direct evaluation of uncertainty in models, parameters and measurements will be viewed through an ill-posed inverse problem and we will demonstrate how incorporating uncertainty can regularize the problem. In particular, we will estimate soil hydraulic properties using two different types of measurements, and incorporate uncertainty due to spatial variation. These estimates can be used over larger scales than those that were measured, and their corresponding uncertainty indicates areas where measurement uncertainty needs to be reduced.

Jodi Mead
Boise State University
Department of Mathematics
jmead@boisestate.edu

MS79
Using Electrochemical Impedance Spectroscopy for Studying Respiration of Anode Respiring Bacteria for Solid Oxide Fuel Cells

Electrochemical impedance spectroscopy (EIS) is a powerful diagnostic technique that involves applying a small AC voltage to an electrode for a range of frequencies. EIS for estimating anode resistances in the study of anode bacteria respiration is of interest. Respiration of the bacteria leads to an electrical current that can be used for various bioenergy applications. Here the focus is on the inverse problem for practical data obtained in solid-oxide fuel cell research.

Rosemary A. Renaut
Arizona State University
School of Mathematical and Statistical Sciences
renaut@asu.edu

MS79
Quantifying Simplification-induced Error using Subspace Techniques

All geophysical models represent a simplification of real-

ity. As a result, the history-matching process can lead to surrogate parameters that compensate for model simplification. This parameter surrogacy may or may not create predictive bias, depending on prediction sensitivity to null and solution space parameter components. The potential for bias indicates the role of history matching is prediction dependent. History-matching-induced predictive bias is analyzed and quantified from a subspace perspective for a physics-based water resource model.

Jeremy White
U.S. Geological Survey
Florida Water Science Center
jwhite@usgs.gov

Joseph Hughes
US Geological Survey
Florida Water Science Center
jdhughes@usgs.gov

MS80
Hybrid Reduced order Modeling for Uncertainty Management in Nuclear Modeling

The speaker will overview reduced order modeling techniques currently used in nuclear reactor design calculations. Reactor calculations are very complex given that nature of the physics governing their behavior and their heterogeneous design. Reduced order modeling is therefore required to allow engineers to carry out design calculations on a routine basis. In doing so, the fidelity of the calculations must be preserved. When used to perform uncertainty quantification, sensitivity analysis, or data assimilation, additional reduction is necessary since these analyses require many executions of the models. The speaker has developed hybrid statistical deterministic reduction techniques to enable the execution of these analysis on a routine basis. He will give a quick overview of reduction techniques used in best-estimate reaction calculations, then focus in depth on reduction algorithms he developed to perform sensitivity and uncertainty analyses.

Hany S. Abdel-Khalik
North Carolina State Univ.
abdelkhalik@ncsu.edu

MS80
Sparse Interpolatory Reduced-Order Models for Simulation of Light-Induced Molecular Transformations

We describe an efficient algorithm for using a quantum-chemistry simulator to drive a gradient descent algorithm. Our objective is to model light-induced molecular transformations. The simulator is far too expensive and the design space too high-dimensional for the simulator to be used directly to drive the dynamics. We begin by applying domain-specific knowledge to reduce the dimension of the design space. Then we use sparse interpolation to model the energy from the quantum code on hyper-cubes in configuration space, controlling the volume of the hyper-cubes both to maintain accuracy and to avoid failure of the quantum codes internal optimization. We will conclude the presentation with some examples that illustrate the algorithm's effectiveness.

Carl T. Kelley
North Carolina State Univ
Department of Mathematics

tim_kelley@ncsu.edu

David Mokrauer
Dept of Mathematics
NC State University
dsmokrau@ncsu.edu

MS80
Intrusive Analysis for Uncertainty Quantification of Simulation Models

We develop intrusive, hybrid uncertainty quantification methods applicable to modern, high-resolution simulation models. We seek to construct surrogate models of uncertainty by augmenting knowledge of the model with results of intrusive analysis, such as Automatic Differentiation. Our toolset now includes a gradient-enhanced regression, stochastic-processes based analysis that provides error bounds and statistical metrics for the prior regression model, and a framework for the use of reduced, lower-fidelity approximations to effectively describe uncertainties in the model.

Oleg Roderick
Argonne National Laboratory
roderick@mcs.anl.gov

PP1
A Statistical Decision-Theoretic Approach to Dynamic Resource Allocation for a Self-Aware Unmanned Aerial Vehicle

For inference and prediction tasks, it is typical for decision-makers to have available to them several different numerical models as well as experimental data. Our statistical decision-theoretic approach to dynamic resource allocation seeks to exploit optimally all available information by selecting models and data with the appropriate fidelity for the task at hand. We demonstrate our approach on the online prediction of flight capabilities for a self-aware unmanned aerial vehicle.

Doug Allaire, Karen E. Willcox
Massachusetts Institute of Technology
dallaire@mit.edu, kwillcox@MIT.EDU

PP1
Computational Reductions in Stochastically Driven Neuronal Models with Adaptation Currents

The complexity of stochastic, conductance-based neuronal network dynamics has motivated several computational reductions to the Hodgkin-Huxley neuron model. These reductions, however, rarely generalize to neurons containing realistic adaptive ionic currents. Using several measures of robustness and network simulations, we show the modeling algorithm described in this talk achieves the goals of attaining accuracy and efficiency while producing a modeling scheme general enough for modeling a wide array of specialized neuronal dynamics.

Victor Barranca
Rensselaer Polytechnic Institute
barrav@rpi.edu

Gregor Kovacic
Rensselaer Polytechnic Inst

Dept of Mathematical Sciences
kovacg@rpi.edu

David Cai
New York University
Courant institute
cai@cims.nyu.edu

PP1
Propagating Arbitrary Uncertainties Through Models Via the Probabilistic Collocation Method

Nonintrusive methods for propagating uncertainty in simulations have been introduced in recent times. Some of these methods use polynomial chaos expansions which can be used with many standard statistical distributions based on the Askey scheme. This work describes an efficient method for propagating arbitrary distributions through forward models based on application of the standard recurrence relation for generating orthogonal polynomials. The method is demonstrated in the context of eddy-current nondestructive evaluation.

Matthew Cherry
University of Dayton Research Institute
matthew.cherry.ctr@wpafb.af.mil

Jeremy Knopp
Air Force Research Laboratory
Jeremy.Knopp@wpafb.af.mil

PP1
A Predictive Model for Geographic Statistical Data

Any planar map may be transformed into a graph. If we consider each country to be represented by a vertex (or node), if they are adjacent they will be joined by an edge. To consider how trends migrate across boundaries, we obtain relevant measures of the statistic we want to consider; namely, the index of prevalence, and the index of incidence. We define a cycle by a given unit of time, usually a year. We then propose various alternate equations whereby, by parametrizing various variables, such as population size, birth rate, death rate, and rate of immigration/emigration, we calculate a new index of prevalence/index of incidence, for the next cycle. For a given data set, each statistic we consider may propagate by a different equation, and/or a different set of parameters; this will be determined empirically. What we are proposing is, technically, to model how a discrete stochastic process propagates geographically, according to geographical proximity. Very often, statistics that depend on geographical proximity are tabulated by variables that are not; i.e., alphabetically. Such a predictive model would be relevant in areas such as public health; and/or crime mapping, for law enforcement purposes. We present an application using a GIS (geographic information system).

Jorge Diaz-Castro
University of P.R. School of Law
University of P.R. at Rio Piedras
transcripciones@mail.com

PP1
A Stochastic Collocation Method Combined with a Reduced Basis Method to Compute Uncertainties in the Sar Induced by a Mobile Phone

A reduced basis method is introduced to deal with a stochastic problem in a numerical dosimetry application in which the field solutions are computed using an iterative solver. More precisely, the computations already performed are used to build an initial guess for the iterative solver. It is shown that this approach significantly reduces the computational cost.

Mohammed Amine Drissaoui
Laboratoire AMPERE
Amine.Drissaoui@ec-lyon.fr

PP1
Uncertainty Quantification for Hydromechanical Coupling in Three Dimensional Discrete Fracture Network

Fractures and fracture networks are the principle pathways for migration of water, heat and mass in geothermal systems, oil/gas reservoirs, sequestrated CO_2 leakages. We investigate the impact of parameter uncertainties of the PDFs that characterize discrete fracture networks on the hydromechanical response of the system. Numerical results of first, second and third moments, normalized to a base case scenario, are presented and integrated into a probabilistic risk assessment framework. (Prepared by LLNL under Contract DE-AC52-07NA27344)

Souheil M. Ezzedine, Frederick Ryerson
LLNL
ezzedine1@llnl.gov, ryerson@llnl.gov

PP1
Random and Regular Dynamics of Stochastically Driven Neuronal Networks

Dynamical properties of and uncertainty quantification in Integrate-and-Fire neuronal networks with multiple time scales of excitatory and inhibitory neuronal conductances driven by random Poisson trains of external spikes will be discussed. Both the asynchronous regime in which the network spikes arrive at completely random times and the synchronous regime in which network spikes arrive within periodically repeating, well-separated time periods, even though individual neurons spike randomly will be presented.

Pamela B. Fuller
Rensselaer Polytechnic Institute
Fullep@rpi.edu

PP1
Calibration of Computer Models for Radiative Shock Experiments

POLAR experiments aimed to mimic the astrophysical accretion shock formation in laboratory using high-power laser facilities. The dynamics and the main physical properties of the radiative shock produced by the collision of the heated plasma with a solid obstacle have been characterised on recent experiments and compared to radiation hydrodynamic simulations. This poster will present the statistical method based on Bayesian inference used to calibrate the main unknown parameters of the simulation and to quantify the model uncertainty.

Jean Giorla

Commissariat à l'Energie Atomique, France
jean.giorla@cea.fr

E. Falize, C. Busschaert, B. Loupias
CEA/DAM/DIF, F-91297, Arpajon, France
emeric.falize@cea.fr, clotilde.busschaert@cea.fr,
berenice.loupias@cea.fr

M. Koenig, A. Ravasio, A. Dizière
Laboratoire LULI, Ecole Polytechnique, Palaiseau, France
michel.koenig@polytechnique.fr,
alessandra.ravasio@polytechnique.fr,
alexandra.diziere@polytechnique.edu

Josselin Garnier
Universite Paris 7
garnier@math.jussieu.fr

C. Michaut
LUTH, Observatoire de Paris, Meudon, France
claire.michaut@obspm.fr

PP1
Regional Climate Model Ensembles and Uncertainty Quantification

One goal of the North American Regional Climate Change Assessment Program (NARCCAP) is to better understand regional climate model output and the impact of the boundary conditions provided by the global climate model, the regional climate model itself, and interaction between the two. This poster will outline a statistical framework for quantifying temperature output and the associated uncertainty both spatially and temporally. The aim is to understand the contributions of each model type and how those contributions vary over space.

Tamara A. Greasby
National Center for Atmospheric Research
tgreasby@ucar.edu

PP1
Multiple Precision, Spatio-Temporal Computer Model Validation using Predictive Processes

The Lyon-Fedder-Mobarry (LFM) global magnetosphere model is a computer model used to study physical processes in the magnetosphere and ionosphere. Given a set of input values and solar wind data, the LFM model numerically solves the magnetohydrodynamic equations and outputs a spatio-temporal field of ionospheric energy. The LFM model has the benefit of being able to be run at multiple precisions (with higher precisions more closely representing true ionospheric conditions at the cost of computation). This work focuses on relating the multiple precision output from the LFM model to field observations of ionospheric energy. Of particular interest here are the input settings (and their uncertainties) of the LFM model which most closely match the field observations. A low rank spatio-temporal statistical LFM model emulator is constructed using predictive processes. The emulator borrows strength across the multiple precisions of the LFM model to calibrate the input variables to field observations. In this way, the less computationally demanding yet lower precision models are leveraged to provide estimates of the higher precision LFM model output.

Matthew J. Heaton

National Center for Atmospheric Research
heaton@ucar.edu

Stephan Sain
Institute for Mathematics Applied to Geosciences
National Center for Atmospheric Research
ssain@ucar.edu

William Kleiber, Michael Wiltberger
National Center for Atmospheric Research
wkleiber@ucar.edu, wiltbemj@ucar.edu

Derek Bingham
Dept. of Statistics and Actuarial Science
Simon Fraser University
dbingham@cs.sfu.ca

Shane Reese
Brigham Young University
reese@stat.byu.edu

PP1
Variance Based Sensitivity Analysis of Epidemic Size to Network Structure

I demonstrate the use of global sensitivity analysis to study the dependence of epidemic growth on the structure of the underlying network. These networks model the social interactions and migration patterns of individuals susceptible to a disease. Variance based sensitivity indices are shown to indicate quantities in the structure of these networks that determine the behaviour of epidemics.

Kyle S. Hickmann, James (Mac) Hyman, John E. Ortmann
Tulane University
khickma@tulane.edu, mhyman@tulane.edu, jortmann@tulane.edu

PP1
Autoregressive Model for Real-Time Weather Prediction and Detecting Climate Sensitivity

We propose reduced stochastic models with nonlinear terms replaced by autoregressive linear stochastic model in Fourier space for filtering and for climate modeling. Using the Lorenz-96 model as a test bed, we show that this reduced filtering strategy is computationally cheap and provides more accurate filtered solutions than current methods. The potential of application of this autoregressive model to study climate sensitivity using the Fluctuation-Dissipation Theorem (FDT) is also addresses.

Emily L. Kang
Department of Mathematical Sciences
University of Cincinnati
kangel@ucmail.uc.edu

John Harlim
Department of Mathematics
North Carolina State University
jharlim@ncsu.edu

PP1
A Split Step Adams Moulton Milstein Method for

Stiff Stochastic Differential Equations

A split-step method for solving Itō stochastic differential equations (SDEs) is presented. The method is based on Adams Moulton Formula for stiff ordinary differential equations and modified for use on stiff SDEs which are stiff in both the deterministic and stochastic components. Its order of convergence is proved and stability regions are displayed. Numerical results show the effectiveness of the method in the path-wise approximation of SDEs and its' capability to deal with uncertainty.

Abdul M. Khaliq
Middle Tennessee State University
Department of Mathematical Sciences
akhaliq@mtsu.edu

David A. Voss
Western Illinois University
d-voss1@wiu.edu

PP1

Computer Model Calibration with High and Low Resolution Model Output for Spatio-Temporal Data

We discuss a framework for computer model calibration based on low and high resolution model output for large spatio-temporal datasets. The physical model in use is a coupled magnetohydrodynamical model for solar storms occurring in Earth's upper atmosphere. The statistical model is informed by known physical equations and is tailored to large datasets. Given initial runs of the computer model, we propose a sequential design based on Expected Improvement.

William Kleiber
National Center for Atmospheric Research
wkleiber@ucar.edu

Stephan Sain
Institute for Mathematics Applied to Geosciences
National Center for Atmospheric Research
ssain@ucar.edu

Michael Wiltberger
National Center for Atmospheric Research
wiltbemj@ucar.edu

Derek Bingham
Dept. of Statistics and Actuarial Science
Simon Fraser University
dbingham@cs.sfu.ca

Shane Reese
Brigham Young University
reese@stat.byu.edu

PP1

Goal-Oriented Statistical Inference

In many applications statistical inference is utilized for model identification before simulations are conducted to predict outputs of interest. Our goal-oriented approach to inference automatically targets parameter modes required to make predictions. In the linear Gaussian case, the mean and covariance of the posterior predictive are obtained by inferring many fewer parameter modes than an unmodi-

fied approach. This method could pave the way for efficient Markov chain Monte Carlo in the high-dimensional parameter setting.

Chad E. Lieberman
MIT
celieber@mit.edu

Karen E. Willcox
Massachusetts Institute of Technology
kwillcox@MIT.EDU

PP1

Uncertainty in Model Selection in Remote Sensing

The model choice problem arise in the context of estimating the total amount of atmospheric aerosols using satellite measurements. Modeling uncertainty related to unknown aerosol type is taken into account when assessing uncertainty in aerosol products using Bayesian model selection tools. In this work, uncertainty modeling is comprised of measurement uncertainty estimates, uncertainty in aerosol models, and uncertainty in model selection. Illustrating and quantifying modeling uncertainty gives valuable information to algorithm developers and users.

Anu Määttä, Marko Laine, Johanna Tamminen
Finnish Meteorological Institute
anu.maatta@fmi.fi, marko.laine@fmi.fi,
johanna.tamminen@fmi.fi

PP1

Multifidelity Approach to Variance Reduction in Monte Carlo Simulation

Engineers often have a suite of numerical models at their disposal to simulate a physical phenomenon. For uncertainty propagation, we present an approach that utilizes information from inexpensive, low-fidelity models to reduce the variance of the Monte Carlo estimator of an expensive, high-fidelity model. For a given computational budget, we demonstrate that our approach can produce more accurate estimation of the statistics of interest than regular Monte Carlo simulation.

Leo Ng, Karen E. Willcox
Massachusetts Institute of Technology
leo_ng@mit.edu, kwillcox@MIT.EDU

PP1

Local Sensitivity Analysis of Stochastic Systems with Few Samples

We estimate local sensitivity of predicted quantities in stochastic models with respect to input parameters by minimizing the Lp residual of linear hyperplanes fit through sparse multidimensional output. We analyze how the number of function evaluations necessary for reliable estimates for the sensitivity indices depends upon the Lp norm $(0 < p < 2)$ used and how the optimal Lp norm can reduce the number of function evaluations necessary for the sensitivity analysis. We apply this method to an epidemic model.

John E. Ortmann, James (Mac) Hyman, Kyle S. Hickmann
Tulane University
jortmann@tulane.edu, mhyman@tulane.edu,
khickma@tulane.edu

PP1

Worst Case Scenario Analysis Applied to Uncertainty Quantification in Electromagnetic Simulations

The input parameters of models used for the simulation of technical devices exhibit uncertainties, e.g., due to the manufacturing process. Whenever their probability distribution is unknown, a worst case scenario analysis [Babuška et al. (2005)] is appealing, potentially requiring little numerical effort. Based on sensitivity analysis techniques, the quantification of uncertainty due to variations in geometry, material distribution and sources will be discussed for electromagnetic problems within the finite element method.

Ulrich Roemer
Technische Universitaet Darmstadt
Institut fuer Theorie Elektromagnetischer Felder
roemer@temf.tu-darmstadt.de

Stephan Koch
Institut fuer Theorie Elektromagnetischer Felder
Technische Universitaet Darmstadt
koch@temf.tu-darmstadt.de

Thomas Weiland
Institut fuer Theorie Elektromagnetischer Felder, TEMF
Technische Universitaet Darmstadt
weiland@temf.tu-darmstadt.de

PP1

Constructive and Destructive Correlation Dynamics in Simple Stochastic Swimmer Models

Micro-swimming organisms usually can be classified into two groups based on their method of propulsion: pushers and pullers. Experimental data as well as numerical simulations point towards much larger orientational correlations for suspensions of pushers compared to pullers. I will discuss an analytical mean field theory for a simplified swimmer model that captures two body interactions and can help lead to an understanding of the above observations.

Kajetan Sikorski
Rensselaer Polytechnic Institute
Department of Mathematical Sciences
sikork@rpi.edu

PP1

Preserving Positivity in Pc Approximations Via Weighted Pc Expansions

The preservation of the positivity of the solution in dynamical systems is important in a wide range of applications. When working with polynomial chaos (PC) approximations, the positivity can be lost after the truncation of the PC expansion. We show that the introduction of weights in the PC approximations solves this problem for a wide range of polynomial systems. We present sufficient conditions for the weights and an algorithm that allows determining these weights.

Faidra Stavropoulou, Josef Obermaier
Helmholtz Zentrum Muenchen
faidra.stavropoulou@mytum.de,
josef.obermaier@helmholtz-muenchen.de

PP1

Visualization of Uncertainty: Standard Deviation and Pdf's

Uncertainty can be expressed as an error bar (ie standard deviation) or a distribution. Except for the simplest cases, concurrent visualization of uncertainty and underlying value, uncertainty remains un-visualized. We present a method to display scalar uncertainty based on tessellating the field of uncertainty density into cells containing nearly equal uncertainty. We present a method for segmenting a field of node based probability distributions into meaningful features. We use climate data to illustrate the concepts.

Richard A. Strelitz
Los Alamos Naitional Laboratory
Los Alamos National Laboratory
strelitz@lanl.gov

PP1

How Typical Is Solar Energy? A 6 Year Evaluation of Typical Meteorological Year Data (TMY3)

The US solar industry makes bets on system performance using NRELs typical meteorological year data (TMY3). TMY3 is a 1-year dataset of typical solar irradiance and other meteorological elements used for simulation of solar power production. Irradiance naturally varies from TMY3 temporally and geographically, thus creating risk. Using data from NOAAs Surface Radiation Network (SurfRad), 6-years of irradiance observations were analyzed. Statistically comparing SurfRad against TMY3 quantified temporal and geographic uncertainty in typical solar irradiance.

Matthew K. Williams, Shawn Kerrigan
Locus Energy
matthew.williams@locusenergy.com,
shawn@locusenergy.com

PP1

Second-Order Probability for Error Analysis in Numerical Computation

It is difficult to quantify the uncertainty for numerical computation because computational error are deeply affected by many epistemic uncertainty variables. The best known methods for estimating computational error are Richardson extrapolation(RE) and generalized RE. However, it only estimate descretization error. In this paper we propose second-order probability method for error analysis in numerical computation. This method can provide integrated error analysis for all error sources and quantify measurement uncertainty of numerical computation error.

Hua Chen, Yingyan Wu, Shudao Zhang, Haibing Zhou, Jun Xiong
Institute of Applied Physics and Computational Mathematics
chen_hua@iapcm.ac.cn,   wu_yingyan@iapcm.ac.cn,
zhang_shudao@iapcm.ac.cn,   zhou_haibing@iapcm.ac.cn,
xiong_jun@iapcm.ac.cn