**Final Program and Abstracts** 

# SIAM Conference on UNCERTAINTY QUANTIFICATION

March 31-April 3, 2014 Hyatt Regency Savannah Savannah, Georgia, USA

Sponsored by the SIAM Activity Group on Uncertainty Quantification (SIAG/UQ)

The SIAM Activity Group on Uncertainty Quantification (SIAG/UQ) fosters activity and collaboration on all aspects of the effects of uncertainty and error on mathematical descriptions of real phenomena. It seeks to promote the development of theory and methods to describe quantitatively the origin, propagation, and interplay of different sources of error and uncertainty in analysis and predictions of the behavior of complex systems, including biological, chemical, engineering, financial, geophysical, physical and social/political systems. The SIAG/UQ serves to support interactions among mathematicians, statisticians, engineers, and scientists working in the interface of computation, analysis, statistics, and probability.

The activity group sponsors the biennial SIAM Conference on Uncertainty Quantification and maintains a website, a member directory, and an electronic mailing list.

This conference is being held in cooperation with the American Statistical Association (ASA), GAMM Activity Group on Uncertainty Quantification (GAMM AG UQ), and American Geophysical Union (AGU).

# siam

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### **SIAM Registration Desk**

The SIAM registration desk is located in the Registration Booth on the  $2^{nd}$  floor. It is open during the following hours:

Sunday, March 30 5:00 PM – 8:00 PM

Monday, March 31 7:00 AM – 5:00 PM

Tuesday, April 1 7:30 AM - 5:00 PM

Wednesday, April 2 7:30 AM - 5:00 PM

Thursday, April 3 7:30 AM - 5:00 PM

### **Hotel Address**

hotels/index.jsp

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List current February 2014.

## **Funding Agencies**

SIAM and the Conference Organizing Committee wish to extend their thanks and appreciation to the U.S. National Science Foundation and the U.S. Department of Energy (DOE), Office of Science, for their support of this conference.





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If you are a SIAM member, it only costs \$10 to join the SIAM Activity Group on Uncertainty Quantification (SIAG/ UQ). As a SIAG/UQ member, you are eligible for an additional \$10 discount on this conference, so if you paid the SIAM member rate to attend the conference, you might be eligible for a free SIAG/UQ membership. Check at the registration desk.

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## **Registration Fee Includes**

- Admission to all technical sessions
- Business Meeting (open to SIAG/UQ members)
- Coffee breaks daily
- Poster Session
- Room set-ups and audio/visual equipment
- Welcome Reception and Poster Session

## Job Postings

Please check with the SIAM registration desk regarding the availability of job postings or visit *http://jobs.siam.org*.

## Important Notice to Poster Presenters

The poster session is scheduled for Monday, March 31 at 8:00 PM. Poster presenters are requested to set up their poster material on the provided 4' x 8' poster boards in the Harborside East Room, located on the River Street Level, between the hours of 2:00 PM and 8:00 PM on Monday. All materials must be posted by Monday, March 31 at 8:00 PM, the official start time of the session. Poster displays must be removed by 10:00 PM. Posters remaining after this time will be discarded. SIAM is not responsible for discarded posters.

## SIAM Books and Journals

Display copies of books and complimentary copies of journals are available on site. SIAM books are available at a discounted price during the conference. If a SIAM books representative is not available, completed order forms and payment (credit cards are preferred) may be taken to the SIAM registration desk. The books table will close at 11:30 AM on Thursday, April 3.

## **Tabletop Displays**

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## Comments?

Comments about SIAM meetings are encouraged! Please send to:

Cynthia Phillips, SIAM Vice President for Programs (*vpp@siam.org*).

## Get-togethers

- Welcome Reception Sunday, March 30
  6:00 PM - 8:00 PM
- Poster Session Monday, March 31
  8:00 PM - 10:00 PM



Business Meeting
(open to SIAG/UQ members)
Tuesday, April 1

8:00 PM - 8:45 PM

*Complimentary beer and wine will be served.* 

## Please Note

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Audio and video recording of presentations at SIAM meetings is prohibited without the written permission of the presenter and SIAM.

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SIAM is promoting the use of social media, such as Facebook and Twitter, in order to enhance scientific discussion at its meetings and enable attendees to connect with each other prior to, during and after conferences. If you are tweeting about a conference, please use the designated hashtag to enable other attendees to keep up with the Twitter conversation and to allow better archiving of our conference discussions. The hashtag for this meeting is #SIAMUQ14.

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## **Minitutorials**

\*\*All Minitutorials will take place in Ballroom  $A - 2^{nd}$  Floor \*\*

Monday, March 31

### 9:30 AM - 11:30 AM

# MT1: Multi-resolution Spatial Methods for Large Data Sets

Typically, a spatial analysis is necessary for calibration between geophysical models and observations but also has more general application for the analysis of computer experiments. Standard statistical methods break when applied to large data sets and so alternative approaches are needed that balance changes to the statistical models for increases in computational efficiency. By expanding the field in a flexible set of basis functions it is possible to entertain multi-resolution and nonstationary spatial models.

Organizer and Speaker:

**Douglas Nychka**, National Center for Atmospheric Research, USA

2:00 PM - 4:00 PM

### MT2: A Posteriori Error Estimates for Statistical Computations with Differential Equations with Stochastic Parameters

A posteriori error estimates for numerical solutions of differential equations precisely quantify the effects of different sources of discretization error on the accuracy of computed information. We will present the ingredients of a posteriori analysis, including an extension to statistical information computed from differential equations with stochastic parameters. We will use the estimates as the basis for a selective computational approach to efficiently distribute computational resources to control various sources of stochastic and deterministic errors.

Organizer and Speaker: **Don Estep,** Colorado State University, USA



Throughout 2014, the ASA will look back at our history, explore our present, and learn about future plans for our association!



www.amstat.org/asa175

## **Minitutorials**

\* \*All minitutorials will take place in Ballroom A-2nd Floor\*\*

Tuesday, April 1

### 9:30 AM - 11:30 AM

### MT3: Reduced Order Methods for Modelling and Computational Reduction in UQ Problems

We present the state of the art of some reduced order methods for modelling and computational reduction, adapted and developed for uncertainty quantification problems. We first focus on forward problems, then we deal with inverse problems, in particular with optimal control problems. Proper adaptation of reduced basis method and related techniques is introduced. A special attention is devoted to robust optimization under uncertainty.

This session is designed to complement MS45: Inverse Problems in Cardiovascular Mathematics.

Organizer and Speaker:

**Gianluigi Rozza,** SISSA, International School for Advanced Studies, Trieste, Italy

#### 2:00 PM - 4:00 PM

### MT4: VV&EQ and Reproducible Computational Science

This minitutorial will outline relationships between Validation and Verification as understood in the scientific computing community, and Reproducibility as understood across the computational sciences. It will also address notions of inherent uncertainty and sources of error when reproducing computational findings, and trace these back to the established concept of uncertainty quantification.

This session is designed to complement MS42: The Reliability of Computational Research Findings: Reproductible Research, Uncertainty Quantification, and Verification & Validation.

Organizer and Speaker: Victoria Stodden, Columbia University, USA

# Uncertainty Quantification Theory, Implementation, and Applications



## Ralph C. Smith

The field of uncertainty quantification is evolving rapidly because of increasing emphasis on models that require quantified uncertainties for large-scale applications, novel algorithm development, and new computational architectures that facilitate implementation of

these algorithms. Uncertainty Quantification: Theory, Implementation, and Applications provides readers with the basic concepts, theory, and algorithms necessary to quantify input and response uncertainties for simulation models arising in a broad range of disciplines.

The book begins with a detailed discussion of applications where uncertainty quantification is critical for both scientific understanding and policy. It then covers concepts from probability and statistics, parameter

selection techniques, frequentist and Bayesian model calibration, propagation of uncertainties, quantification of model discrepancy, surrogate model construction, and local and global sensitivity analysis. The author maintains a complementary web page where readers can find data used in the exercises and other supplementary material.

Uncertainty Quantification: Theory, Implementation, and Applications includes a large number of definitions and examples that use a suite of relatively simple models crucial to understanding concepts that cover a range of disciplines, numerous references to current and open research issues, and exercises that illustrate basic concepts and guide readers through the numerical implementation of algorithms for prototypical problems. It also features a wide range of applications, including weather and climate models, subsurface hydrology and geology models, nuclear power plant design, and models for biological phenomena, along with recent advances and topics that have appeared in the research literature within the last 15 years, including aspects of Bayesian model calibration, surrogate model development, parameter selection techniques, and global sensitivity analysis.

**Audience** – The text is intended for advanced undergraduates, graduate students, and researchers in mathematics, statistics, operations research, computer science, biology, science, and engineering. It can be used as a textbook for one- or two-semester courses on uncertainty quantification or as a resource for researchers in a wide array of disciplines. A basic knowledge of probability, linear algebra, ordinary and partial differential equations, and introductory numerical analysis techniques is assumed.

**About the Authors** – **Ralph C. Smith** is a Professor of Mathematics and Associate Director of the Center for Research in Scientific Computation at North Carolina State University.

2013 · xviii + 383 pages · Hardcover · 978-1-611973-21-1 List \$74.00 · SIAM Member \$51.80 · Attendee \$59.20 · Order Code CS12



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Preface; Notation; Acronyms and Initialisms Chapter 1: Introduction Chapter 2: Large-Scale Applications Chapter 3: Prototypical Models Chapter 4: Fundamentals of Probability, Random Processes, and Statistics Chapter 5: Representation of Random Inputs Chapter 6: Parameter Selection Techniques Chapter 7: Frequentist Techniques for Parameter Estimation Chapter 8: Bayesian Techniques for Parameter Estimation Chapter 9: Uncertainty Propagation in Models Chapter 10: Stochastic Spectral Methods Chapter 11: Sparse Grid Quadrature and Interpolation Techniques Chapter 12: Prediction in the Presence of Model Discrepancy Chapter 13: Surrogate Models Chapter 14: Local Sensitivity Analysis Chapter 15: Global Sensitivity Analvsis Appendix A: Concepts from Functional Analysis Bibliography; Index

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## **Minitutorials**

\* \*All minitutorials will take place in Ballroom A-2nd Floor\*\*

Wednesday, April 2

#### 9:30 AM - 11:30 AM

### MT5: Estimation of Prediction Uncertainties in Oil Reservoir Simulation using Bayesian and Proxy Modeling Techniques

Subsurface uncertainties have a large impact on oil & gas production forecasts. Underestimation of prediction uncertainties therefore presents a high risk to investment decisions for facility designs and exploration targets. The complexity and computational cost of reservoir simulation models often defines narrow limits for the number of simulation runs used in related uncertainty quantification studies. In this mini tutorial we will look into workflow designs and methods that have proven to deliver results in industrial reservoir simulation workflows. Combinations of automatic proxy modeling, MCMC and Bayesian approaches for estimating prediction uncertainties are presented.

Organizer and Speaker:

Ralf Schulze-Riegert, Schlumberger, Norway

2:00 PM - 4:00 PM

### MT6: A Few Elements of Numerical Analysis for Elliptic PDEs with Random Coefficients of lognormal Type

In this minitutorial we will focus on the case of elliptic PDEs with lognormal coefficients, however most ideas are more general. Such coefficients raise several mathematical difficulties : they are neither uniformly bounded from above nor below, they may have low spatial regularity and have nonaffine dependance on the random parameters. We will explain how to establish error estimates, by illustrating this in the cases of the Monte-Carlo method and the stochastic collocation method.

This session is designed to complement MS69: PDEs with Random Coefficients of lognormal Type and Applications to Subsurface Flow.

Organizer and Speaker: Julia Charrier, Aix-Marseille Université,

France

# SIAM Activity Group on Uncertainty Quantification (SIAG/UQ)

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- · Electronic communications about recent developments in your specialty
- Eligibility for candidacy for SIAG/UQ office
- Participation in the selection of SIAG/UQ officers

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## SIAM Conference on UNCERTAINTY QUANTIFICATION

March 31-April 3, 2014 Hyatt Regency Savannah Savannah, Georgia, USA

## **Minitutorials**

\* \*All minitutorials will take place in Ballroom A-2nd Floor\*\*

Thursday, April 3

#### 9:30 AM - 11:30 AM

# MT7: Numerical Analysis for PDEs with Random Inputs

We provide an introduction to numerical methods for Uncertainty Quantification. We start by discussing data parametrization and then we study the implementation and convergence of several methods for forward propagation. To this end, we begin with Monte Carlo and Multi level Monte Carlo sampling and then show the use how to exploit higher solution regularity within L2 projection and discrete L2 projection methods. Throughout the presentation, numerical examples provide insight into the theory.

Organizer and Speaker:

Raul F. Tempone, King Abdullah University of Science & Technology (KAUST), Saudi Arabia

#### 2:00 PM - 4:00 PM

### MT8: Uncertainty Quantification Challenges in High-Performance Scientific Computing

Applying uncertainty quantification methodologies in high performance computing contexts presents numerous challenges such as expensive simulations, complex software frameworks, and the need to leverage advanced computer architecture capabilities. This mini-tutorial will explore techniques for improving performance of UQ methodologies in HPC applications by exposing new dimensions of fine-grained parallelism, improving memory access patterns, and extracting higher-order information, as well as approaches for applying these techniques in large, complex software code bases.

This session is designed to complement MS96: Uncertainty Quantification for Extreme-scale High Performance Computing.

Organizer and Speaker:

**Eric Phipps,** Sandia National Laboratories, USA

## **Invited Plenary Speakers**

\*\* All Invited Plenary Presentations will take place in Ballroom A/B/C - 2nd Floor \*\*

## Monday, March 31

## 8:15 AM - 9:00 AM

IP1 Quantifying Uncertainty in Multiscale Heterogenous Solid Earth Crustal Deformation Data to Improve Understanding of Earthquake Processes

## Andrea Donnellan

NASA Jet Propulsion Laboratory and University of Southern California, USA

## 1:00 PM - 1:45 PM

IP2 Uncertainty Quantification in Nonparametric Regression and III-posed Inverse Problems

## Grace Wahba

University of Wisconsin, Madison, USA

## Tuesday, April 1

## 8:15 AM - 9:00 AM

**IP3** Uncertainty Quantification in Bayesian Inversion

## Andrew Stuart

University of Warwick, United Kingdom

## 1:00 PM - 1:45 PM

**IP4** Evidence-based Treatment of Computer Experiments

## Jerome Sacks

National Institute of Statistical Sciences, USA

## **Invited Plenary Speakers**

\*\* All Invited Plenary Presentations will take place in Ballroom A/B/C - 2nd Floor \*\*

## Wednesday, April 2

## 8:15 AM - 9:00 AM

IP5 Gaussian Process Emulation of Computer Models with Massive Output

### James Berger

Duke University, USA

## 1:00 PM - 1:45 PM

IP6 The Theory Behind Reduced Basis Methods

## Ronald DeVore

Texas A&M University, USA

## Thursday, April 3

## 8:15 AM - 9:00 AM

IP7 Uncertainties Without the Rev. Thomas Bayes

### **Robert Parker** University of California, San Diego, USA

## 1:00 PM - 1:45 PM

**IP8** Recent Advances in Galerkin Methods for Parametric Uncertainty Propagation in Fluid Flow Simulations

> Olivier Le Maître LIMSI-CNRS, France

## Notes

## UQ14 Program

# SIAM Conference on UNCERTAINTY QUANTIFICATION

March 31-April 3, 2014 Hyatt Regency Savannah Savannah, Georgia, USA

## Sunday, March 30

## Registration

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5:00 PM-8:00 PM Room:Registration Booth - 2nd Floor

### Welcome Reception 6:00 PM-8:00 PM



Room:Harborside East - River Street Level

## Monday, March 31

Registration 7:00 AM-5:00 PM Room:Registration Booth - 2nd Floor

## Welcoming Remarks

8:00 AM-8:15 AM Room:Ballroom A/B/C - 2nd Floor Monday, March 31

IP1

Quantifying Uncertainty in Multiscale Heterogenous Solid Earth Crustal Deformation Data to Improve Understanding of Earthquake Processes

8:15 AM-9:00 AM

Room:Ballroom A/B/C - 2nd Floor

Chair: Max Gunzburger, Florida State University, USA

Earthquakes can cause tremendous loss of life and property yet predicting the behavior of earthquake fault systems is exceptionally difficult. The Earth's crust is complex and earthquakes generate at depth, which is problematic for understanding earthquake fault behavior. Geodetic imaging observations of crustal deformation from Global Positioning System (GPS) and Interferometric Synthetic Aperture Radar (InSAR) measurements make it possible to characterize interseismic and aseismic motions, complementing seismic and geologic observations. Earthquake processes and the associated data are multiscale in the spatial and temporal domains making it particularly difficult to quantify uncertainty. Fusing the observations results in better understanding of earthquake processes and characterization of the uncertainties of each data type.

Andrea Donnellan NASA Jet Propulsion Laboratory and University of Southern California, USA

## **Coffee Break**



Room:Regency Foyer and Promenade - 2nd Floor

9:00 AM-9:30 AM

## MT1 Multi-resolution Spatial Methods for Large Data Sets

#### 9:30 AM-11:30 AM

Room:Ballroom A - 2nd Floor Chair: Douglas Nychka, National Center for Atmospheric Research, USA

Typically, a spatial analysis is necessary for calibration between geophysical models and observations but also has more general application for the analysis of computer experiments. Standard statistical methods break when applied to large data sets and so alternative approaches are needed that balance changes to the statistical models for increases in computational efficiency. By expanding the field in a flexible set of basis functions it is possible to entertain multi-resolution and nonstationary spatial models.

*Douglas Nychka*, National Center for Atmospheric Research, USA

### Monday, March 31

## MS1

### Numerical Approximation of Highdimensional Stochastic Equations - Part I of IV

9:30 AM-11:30 AM

Room:Ballroom B - 2nd Floor

#### For Part 2 see MS18

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 are affected by large amounts of uncertainty. For higher accuracy in computational simulations, approximations must increase the number of random variables (dimensions), and expend more effort resolving smooth or even discontinuous behavior within each individual dimension. The resulting explosion in computational effort is a symptom of the efforts effort is a symptom of curse of dimensionality. This minisymposium aims at exploring efforts related to efficient stochastic Galerkin, collocation and Monte Carlo finite element methods, error analysis, anisotropy and adaptive methods, multi-level and multi-resolution analysis, random sampling and sparse grids.

Organizer: Clayton G. Webster Oak Ridge National Laboratory, USA

Organizer: Michael Griebel Universitaet Bonn, Germany

#### 9:30-9:55 Coherence Motivated Monte Carlo Sampling of Sparse Polynomial Chaos Bases

Jerrad Hampton and Alireza Doostan, University of Colorado Boulder, USA

#### 10:00-10:25 A Generalized Clusteringbased Stochastic Collocation Approach for high-dimensional Approximation of PDEs with Random Input Data

*Clayton G. Webster* and Guannan Zhang, Oak Ridge National Laboratory, USA; Max Gunzburger, Florida State University, USA

#### 10:30-10:55 Optimal Polynomial Approximation of Elliptic PDEs with Stochastic Coefficients

*Raul F. Tempone*, King Abdullah University of Science & Technology (KAUST), Saudi Arabia; Fabio Nobile, EPFL, France; Lorenzo Tamellini, EPFL, Switzerland

#### 11:00-11:25 Iterative Solution of Reduced-Order Models for Parameter-Dependent PDEs

Howard C. Elman and Virginia Forstall, University of Maryland, College Park, USA

## MS2 Filtering, Data Assimilation, and UQ - Part I of III

9:30 AM-11:30 AM

Room:Ballroom D - 2nd Floor

#### For Part 2 see MS19

It is recently becoming amenable to take a probabilistic approach to the solution of inverse problems. Solution of the sequential inverse problem, in which the data arrives online, is known as filtering. This subject has enjoyed a long-standing symbiosis between classical and probabilistic approaches. Data Assimilation can be viewed as a bridge between these, built out of the necessity to get solutions to the filtering problem quickly for very high dimensional problems in atmospheric and oceanographic science. This minisymposium aims to bring together experts interested in filtering, Data Assimilation, and UQ to share their latest ideas and project forward.

Organizer: Kody Law King Abdullah University of Science & Technology (KAUST), Saudi Arabia

Organizer: Raul F. Tempone King Abdullah University of Science & Technology (KAUST), Saudi Arabia

#### 9:30-9:55 Accuracy and Stability of The Continuous-Time 3dvar Filter for The Navier-Stokes Equation

Kostas Zygalakis, University of Southampton, United Kingdom; Kody Law, King Abdullah University of Science & Technology (KAUST), Saudi Arabia; Andrew Stuart, University of Warwick, United Kingdom; Dirk Bloemker, Universität Augsburg, Germany

#### 10:00-10:25 Impacts of Varying Spatial and Temporal Density of Observations on Uncertainty with An Atmospheric Ensemble Prediction System

*Jeffrey Anderson*, National Center for Atmospheric Research, USA; Lili Lei, Institute for Mathematics Applied to Geosciences, USA

#### 10:30-10:55 Nested Particle Filters for Sequential Parameter Estimation in Discrete-time Statespace Models

Dan Crisan, Imperial College London, United Kingdom; *Joaquin Miguez*, Universidad Carlos III de Madrid, Spain

#### 11:00-11:25 Quantification of Bayesian Filter Performance for Complex Dynamical Systems through Information Theory

*Michal Branicki*, New York University, USA; Andrew Majda, Courant Institute of Mathematical Sciences, New York University, USA

### Monday, March 31

## MS3 Multi-Parameter Regularization and High-Dimensional Learning

9:30 AM-11:00 AM

#### Room:Ballroom E - 2nd Floor

Making accurate predictions is a crucial factor in many systems. The situation encountered in real-life applications is to have only at disposal incomplete/ rough high-dimensional data, and extracting predictive model from them is an impossible task unless one relies on some a-priori knowledge of properties of expected model. To overcome these fundamental challenges, we incorporate additional information through optimization by means of multiparameter regularization. The main goals of the proposed minisymposium are to set up a new agenda and give a new impulse to the cooperation between approximation and regularization theories within the intrinsic uncertainty of learning process for real-life data.

Organizer: Valeriya Naumova RICAM, Austrian Academy of Sciences, Austria

Organizer: Sergei Pereverzyev RICAM, Austrian Academy of Sciences, Austria

Organizer: Massimo Fornasier Technical University of Munich, Germany

#### 9:30-9:55 Multi-Parameter Regularization for Lifting the Curse of Dimensionality

Valeriya Naumova, RICAM, Austrian Academy of Sciences, Austria

## 10:00-10:25 Not available at time of publication

Ronald DeVore, Texas A&M University, USA

#### 10:30-10:55 Multi-parameter Regularization via an Augmented Approach

Bangti Jin, University of California, Riverside, USA

## MS4

### Gaussian Processes Modelling Uncertainty Layers, from Forward Simulation to Calibration

### 9:30 AM-11:30 AM

#### Room:Ballroom F - 2nd Floor

In large complex systems many layers of modelled uncertainty are necessary through the forward to the inverse problem. We discuss various types of uncertainty and how they can be used together with application to modelling the states with a complex chaotic differential equation model. This session outlines quantifying numerical solver discrepancy in the forward problem, additive model discrepancy on top of the solver output, and the calibration challenges using state and derivative information. The final talk relates all of these steps together showing how the pieces relate and interact, with emphasis on creating a succinct cohesive session.

Organizer: Dave A. Campbell Simon Fraser University, Canada

#### 9:30-9:55 Building Better Simulators: Providing a Probabilistic Representation of Numerical Uncertainty in the Response

*Oksana A. Chkrebtii* and Dave A. Campbell, Simon Fraser University, Canada; Mark Girolami and Ben Calderhead, University College London, United Kingdom

#### 10:00-10:25 Calibration in the Presence of Model Discrepancy

Jenny Brynjarsdottir, Case Western Reserve University, USA; Anthony O'Hagan, University of Sheffield, United Kingdom

#### 10:30-10:55 Model Calibration with Complex Differential Equation Constraints

Matthew T. Pratola, Ohio State University, USA

#### 11:00-11:25 Parameter Calibration Accounting for Multiple Sources of Modeling Uncertainty

Dave A. Campbell, Simon Fraser University, Canada; Jenny Brynjarsdottir, Case Western Reserve University, USA; Oksana A. Chkrebtii, Simon Fraser University, Canada; Matthew T. Pratola, Ohio State University, USA

### Monday, March 31

## MS5

## Uncertainty Quantification in Earth System Modeling, Observation, and Prediction - Part I of III

9:30 AM-11:30 AM

Room: Verelst Room - 2nd Floor

#### For Part 2 see MS13

Uncertainty quantification (UQ) for predicting the evolution of the earth system using limited observations for both model development and testing presents challenges to science, mathematics, statistics, and computation. The goal of the minisymposium is to provide a forum for these diverse communities to discuss ideas that will advance confidence in model predictions of the earth system. We are open to any topic that advances this goal including the estimation and representation of low and high dimensional uncertainties in single or multiple earth system components, emulation of physicsbased numerical models, and use of new approaches to information theoretic metrics.

Organizer: Guang Lin Pacific Northwest National Laboratory, USA

Organizer: Charles Jackson University of Texas at Austin, USA

Organizer: James Gattiker Los Alamos National Laboratory, USA

#### 9:30-9:55 Assessing High-Dimensional Space and Field Dependencies Between Modeled and Observed Climate Data

*Alvaro Nosedal*, University of New Mexico, USA; Charles Jackson, University of Texas at Austin, USA; Gabriel Huerta, University of New Mexico, USA

#### 10:00-10:25 Joint Parameter Exploration of Land Surface and Atmospheric Response to Greenhouse Gas Forcing in Cesm1-Cam5

Ben Sanderson, National Center for Atmospheric Research, USA

continued in next column

#### 10:30-10:55 Impact of Model Resolution for Regional Climate Experiments

Stephan Sain, National Center for Atmospheric Research, USA

#### 11:00-11:25 Applications of Machine Learning to Climate Model UQ

Donald D. Lucas, Lawrence Livermore National Laboratory, USA

## MS6

### UQ Methods in Lowdimensional Subspaces for Turbulent Dynamical Systems - Part I of III

9:30 AM-11:30 AM

Room: Percival Room - 2nd Floor

#### For Part 2 see MS14

Turbulent dynamical systems are characterized by both a large dimensional phase space and a large dimension of instabilities. The existence of these persistent or intermittent instabilities is associated with strong energy transfers between dynamical components that lead to broad energy spectra and strongly non-Guassian statistics. This minisymposium focuses on efficient uncertainty quantification methods designed to provide higherorder statistical information for quantities that 'live' in low-dimensional spaces while they still respect the complex dynamical features connected with the turbulent character of these systems.

Organizer: Themistoklis Sapsis Massachusetts Institute of Technology, USA

Organizer: Andrew Majda Courant Institute of Mathematical Sciences, New York University, USA

#### 9:30-9:55 Goal-oriented Probability Density Function Methods for Uncertainty Quantification

Daniele Venturi and George E. Karniadakis, Brown University, USA

#### 10:00-10:25 Statistically Accurate Low Order Models for Uncertainty Quantification in Turbulent Dynamical Systems

*Themistoklis Sapsis*, Massachusetts Institute of Technology, USA; Andrew Majda, Courant Institute of Mathematical Sciences, New York University, USA

#### 10:30-10:55 Multiscale Filtering with Superparameterization

Ian Grooms, New York University, USA

#### 11:00-11:25 Modeling Uncertainty in Chaos and Turbulence Using Polynomial Chaos and Least Squares Shadowing

*Qiqi Wang*, Massachusetts Institute of Technology, USA; Paul Constantine, Colorado School of Mines, USA

#### Monday, March 31

## MS7 Uncertainty Quantification for Ice Sheet Models

9:30 AM-11:30 AM

Room:Savannah Room - Lobby Level

Understanding the dynamics of polar ice sheets is critical for projections of future sea level rise. Yet, there remain large uncertainties in the inputs of models that describe present and future evolutions of ice sheets, ice shelves or glaciers. These uncertainties can be due to unknown model parameters, noise in the observations, uncertain initial and boundary conditions, or uncertain geometry. This session is intended to present recent developments in uncertainty quantification methods for forward propagation of uncertainty in ice sheet models, as well as for the solution of inverse ice sheet problems.

Organizer: Noemi Petra University of Texas at Austin, USA

Organizer: Omar Ghattas University of Texas at Austin, USA

Organizer: Georg Stadler University of Texas at Austin, USA

#### 9:30-9:55 Representation of Thwaites Glacier Bed Uncertainty in Modeling Experiments

Charles Jackson, University of Texas at Austin, USA

## 10:00-10:25 Quantifying Uncertainties in Ice Sheet Paleo-Thermometry

Andrew Davis, Patrick Heimbach, and Youssef M. Marzouk, Massachusetts Institute of Technology, USA

#### 10:30-10:55 Sensitivity of Greenland Ice Flow to Errors in Model Forcing, Using the Ice Sheet System Model and the DAKOTA Framework

Nicole-Jeanne Schlegel, Jet Propulsion Laboratory, California Institute of Technology; Eric Larour, California Institute of Technology, USA; Mathieu Morlighem, University of California, Irvine, USA; Helene Seroussi, California Institute of Technology, USA

#### 11:00-11:25 Uncertainty Quantification for Large-Scale Bayesian Inverse Problems with Application to Ice Sheet Models

*Noemi Petra*, James R. Martin, Tobin Isaac, Georg Stadler, and Omar Ghattas, University of Texas at Austin, USA

### Monday, March 31

## MS8 Large-scale Experimental Analysis - Part I of II

9:30 AM-11:30 AM

Room: Plimsoll - Lobby Level

#### For Part 2 see MS25

The traditional methods for design and analysis of experiments are tooled for circumstances where few explanatory variables are available and few observations are possible. Today, these assumptions are often violated in experiments conducted for uncertainty quantification. Examples include scenarios where data are taken from multiple sources, many predictors need to be studied, or the response is very intricate. Many techniques designed under the limited information paradigm are computationally inefficient or even intractable in these data-rich environments. This minisymposium invites contributions that study experimental design and analysis when large numbers of predictors and/or observations are present.

Organizer: Matthew Plumlee Georgia Institute of Technology, USA

Organizer: Peter Qian University of Wisconsin, Madison, USA

#### 9:30-9:55 Optimal Bayesian Experimental Design in the Presence of Model Error

Youssef M. Marzouk and *Chi Feng*, Massachusetts Institute of Technology, USA

#### 10:00-10:25 Model Calibration for Large Computer Experiments

Derek Bingham, Simon Fraser University, Canada; Robert Gramacy, University of Chicago, USA

10:30-10:55 iKriging with Big Data

Peter Qian, University of Wisconsin, Madison, USA

#### 11:00-11:25 Bayesian Inference and Uncertainty Quantification for Computationally Expensive Models using High Dimensional Emulators

David Woods, University of Southampton, United Kingdom; Antony Overstall, University of St. Andrews, United Kingdom; Kieran Martin, Office for National Statistics, United Kingdom

## CP1 Inverse Problems

9:30 AM-11:30 AM

Room: Vernon Room - 2nd Floor

Chair: Vasilios Alexiades, University of Tennessee, Knoxville, USA

## 9:30-9:45 Model Fidelity Effect on Calibration of System Parameters

*Ghina N. Absi* and Sankaran Mahadevan, Vanderbilt University, USA

#### 9:50-10:05 Parameter Identification Via Sensitivity and Optimization

Vasilios Alexiades, University of Tennessee, Knoxville, USA

## 10:10-10:25 Parameter Identification in a Bayesian Setting

Bojana V. Rosic, TU Braunschweig, Germany; Oliver Pajonk, SPT Group GmbH, Germany; Anna Kucerova and Jan Sykora, Czech Technical University, Czech Republic; Hermann Matthies, Technische Universität Braunschweig, Germany

#### 10:30-10:45 Parameter Estimation and Uncertainty Quantification of Coupled Reservoir and Geomechanical Modeling at a Co2 Injection Site

Hongkyu Yoon, Pania Newell, and Bill Arnold, Sandia National Laboratories, USA; Sean McKenna, IBM Research, Ireland; Mario Martinez and Joseph Bishop, Sandia National Laboratories, USA; Steven Bryant, University of Texas at Austin, USA

#### 10:50-11:05 Entropy-Bayesian Inversion of Hydrological Parameters in the Community Land Model Using Heat Flux and Runoff Data

*Zhangshuan Hou* and Maoyi Huang, Pacific Northwest National Laboratory, USA; Jaideep Ray and Laura Swiler, Sandia National Laboratories, USA

#### 11:10-11:25 New Index Theory Based Algorithm for the Gravity Gradiometer Inverse Source Problem

Robert C. Anderson and Jonathan Fitton, National Geospatial-Intelligence Agency, USA

## Monday, March 31

## CP2 Differential Equations and Kalman Filters

9:30 AM-11:10 AM

Room:Sloane Room - 2nd Floor

Chair: Andrea N. Arnold, Case Western Reserve University, USA

#### 9:30-9:45 Quantile Estimation for Numerical Solution of Differential Equations with Random Data

*Fredrik Hellman* and Daniel Elfverson, Uppsala University, Sweden; Donald Estep, Colorado State University, USA; Axel Målqvist, Uppsala University, Sweden

#### 9:50-10:05 Numerical Integration Error-Based Innovation in Ensemble Kalman Filters

Andrea N. Arnold, Daniela Calvetti, and Erkki Somersalo, Case Western Reserve University, USA

#### 10:10-10:25 Convergence of Square Root Ensemble Kalman Filters in the Large Ensemble Limit

Evan Kwiatkowski and Jan Mandel, University of Colorado, Denver, USA

#### 10:30-10:45 4DVAR by Ensemble Kalman Smoother

Jan Mandel, University of Colorado, Denver, USA; Elhoucine Bergou and Serge Gratton, ENSEEIHT, Toulouse, France

#### 10:50-11:05Reduced Variance by Robust Design of Boundary Conditions for a Hyperbolic System of Equations Jan Nordstrom and Markus Wahlsten,

Linköping University, Sweden

## Lunch Break 11:30 AM-1:00 PM

Attendees on their own

## Monday, March 31

## IP2

## Uncertainty Quantification in Nonparametric Regression and III-posed Inverse Problems

1:00 PM-1:45 PM

Room:Ballroom A/B/C - 2nd Floor

Chair: Douglas Nychka, National Center for Atmospheric Research, USA

The problem of recovering useful functional information from discrete heterogenous, scattered, noisy, incomplete observational information and prior assumptions concerning the nature of the desired function is ubiquitous in many fields, including numerical weather prediction and biomedical risk factor modeling. In parallel we have the problem of quantifiying the uncertainty in the functional estimates. We will cast this problem in an applicable, but somewhat abstract form as an optimization problem in a Reproducing kernel Hilbert space and discuss the role of cross validation in the trade offs in combining observational data and prior assumptions in functional estimation as well as in modeling uncertainty in the estimates.

Grace Wahba University of Wisconsin, Madison, USA

Intermission 1:45 PM-2:00 PM

## MT2

## A Posteriori Error Estimates for Statistical Computations with Differential Equations with Stochastic Parameters

#### 2:00 PM-4:00 PM

Room:Ballroom A - 2nd Floor Chair: Don Estep, Colorado State University,

Chair: Don Estep, Colorado State University, USA

A posteriori error estimates for numerical solutions of differential equations precisely quantify the effects of different sources of discretization error on the accuracy of computed information. We will present the ingredients of a posteriori analysis, including an extension to statistical information computed from differential equations with stochastic parameters. We will use the estimates as the basis for a selective computational approach to efficiently distribute computational resources to control various sources of stochastic and deterministic errors.

Don Estep, Colorado State University, USA

## Monday, March 31

## MS9

## Advances in Markov Chain Monte Carlo Methods for Large-scale Inverse Problems - Part I of II

2:00 PM-4:00 PM

Room:Ballroom B - 2nd Floor

#### For Part 2 see MS26

Inverse problems convert indirect measurements into characterizations of parameters of a system. Parameters are typically related to measurements by a system of PDEs, which are expensive to evaluate. Data are often limited and noisy while the unknown parameters of interest are often high dimensional, or infinite dimensional in principle. Solution of the inverse problem can be cast in a Bayesian setting and thus naturally tackled with Markov chain Monte Carlo (MCMC) methods. However, designing scalable and efficient MCMC methods for high dimensional inverse problems poses a significant challenge. This minisymposium presents recent advances in MCMC methods for solving large-scale inverse problems.

Organizer: Tiangang Cui Massachusetts Institute of Technology, USA

Organizer: Kody Law King Abdullah University of Science & Technology (KAUST), Saudi Arabia

Organizer: Youssef M. Marzouk Massachusetts Institute of Technology, USA

2:00-2:25 Posterior Exploration of Inverse Equilibrium Problems Using a New a Gibbs-Like Sampler

*Colin Fox*, University of Otago, New Zealand; Markus Neumayer, Technische Universität, Graz, Austria

#### 2:30-2:55 Dimension Dependence of Sampling Algorithms in Hierarchical Bayesian Inverse Problems

Sergios Agapiou, University of Warwick, United Kingdom; Johnathan M. Bardsley, University of Montana, USA; Omiros Papaspiliopoulos, Universitat Pompeu Fabra, Spain; Andrew Stuart, University of Warwick, United Kingdom

#### 3:00-3:25 Parallel Monte Carlo with a Single Markov Chain

Ben Calderhead, University College London, United Kingdom

#### 3:30-3:55 Multilevel Markov Chain Monte Carlo with Applications in Subsurface Flow

*Robert Scheichl*, University of Bath, United Kingdom; Christian Ketelsen, University of Colorado Boulder, USA; Aretha Teckentrup, University of Bath, United Kingdom

continued in next column

## **MS10 Model-Reduction Techniques for Quantifying** and Controlling Uncertainty

### 2:00 PM-4:00 PM

#### Room:Ballroom D - 2nd Floor

Reduced-order models can significantly reduce the computational cost of simulating dynamical systems and therefore constitute a promising approach for making nonintrusive UQ tractable. Reduced-order models are constructed by 1) projecting the original, full-order model onto a low-dimensional subspace, and 2) introducing other approximations (e.g., empirical interpolation, gappy POD) when nonlinearities are present. This minisymposium describes novel approaches for applying model reduction to UQ problems, as well as techniques for quantifying and controlling the uncertainty introduced by using a reduced-order model in lieu of the full-order model.

Organizer: Kevin T. Carlberg Sandia National Laboratories, USA

Organizer: Drew P. Kouri Sandia National Laboratories, USA

#### 2:00-2:25 Adaptive *h*-refinement for Nonlinear Reduced-order Models with Application to Uncertainty Control

Kevin T. Carlberg and Seshadhri Comandur, Sandia National Laboratories, USA

#### 2:30-2:55 Uncertainty Quantification of Errors from Reduced-Order Models

Martin Drohmann and Kevin T. Carlberg, Sandia National Laboratories, USA

#### 3:00-3:25 Reduced Basis Method and Several Extensions for Uncertainty **Quantification Problems**

Peng Chen and Alfio Quarteroni, École Polytechnique Fédérale de Lausanne, Switzerland; Gianluigi Rozza, SISSA, International School for Advanced Studies, Trieste, Italy

#### 3:30-3:55 Reduced Basis Collocation Methods for Partial Differential Equations with Random Coefficients

Howard C. Elman, University of Maryland, College Park, USA; Oifeng Liao, Massachusetts Institute of Technology, USA

## Monday, March 31

## **MS11 Stochastic Evolution Equations and Exit Problems** - Part I of II

### 2:00 PM-4:00 PM

Room:Ballroom E - 2nd Floor

#### For Part 2 see MS20

This minisymposium explores recent work of exit problems that arise in the context of stochastic evolution equations, drawn from application areas ranging from nonlinear optics to fluid dynamics to climate models. The presence of lowdimensional dynamics mitigates the challenge introduced by the absence of a gradient flow in many of these systems. The exits themselves are rare events. suggesting techniques borrowed from large deviation theory.

Organizer: Richard O. Moore New Jersey Institute of Technology, USA

Organizer: Tobias Schaefer City University of New York, Staten Island, USA

2:00-2:25 Large Deviations and Variational Representations for Infinite **Dimensional Stochastic Systems** Paul Dupuis, Brown University, USA

#### 2:30-2:55 Large Deviations for Stochastic Dynamical Systems Driven by a Poisson Noise

Amarjit Budhiraja, University of North Carolina, Chapel Hill, USA

#### 3:00-3:25 The Minimum Action Method for the Study of Rare Events

Weiging Ren. National University of Singapore and IHPC, Singapore

#### 3:30-3:55 Efficient Computation of Instantons in Complex Systems Tobias Schaefer, City University of New

York, Staten Island, USA

## Monday, March 31

## **MS12**

## Model Form Uncertainty in Modeling, Simulation, and Analysis - Part I of III

2:00 PM-4:00 PM

Room:Ballroom F - 2nd Floor

#### For Part 2 see MS21

Model form uncertainty is one of the earliest and most important sources of uncertainty in the modeling and simulation process, yet it is the least understood and hardest to quantify, because it is often confounded with other uncertainty sources. This minisymposium intends to focus on state-of-the-art methods to quantify model form uncertainty, including probabilistic and non-probabilistic approaches. A clear understanding of these approaches as to what they quantify and how to integrate the quantification of model form uncertainty with other uncertainty sources will make a significant contribution towards assessing and improving the confidence in simulation-based prediction.

Organizer: Yan Wang Georgia Institute of Technology, USA

Organizer: Sankaran Mahadevan Vanderbilt University, USA

Organizer: Laura Swiler Sandia National Laboratories, USA

#### 2:00-2:25 Options for Quantifying **Model Form Uncertainty**

Sankaran Mahadevan, Vanderbilt University, USA

#### 2:30-2:55 Multi-Fidelity Uncertainty **Quantification of Complex Simulation** Models

Oleg Roderick, Mihai Anitescu, and Yulia Peet, Argonne National Laboratory, USA

#### 3:00-3:25 Calibration, Validation, and Model Uncertainty of Coarse-Grained Models of Atomic Systems

Kathryn Farrell, J. Tinsley Oden, Peter Rossky, and Eric Wright, University of Texas at Austin, USA

#### 3:30-3:55 Quantification of Model Form **Uncertainty for Run-Time Optimization** of Simulation-Based Predictions

Martin Drohmann, Khachik Sargsyan, Bert J. Debusschere, Habib N. Najm, Jeremiah Wilke, and Gilbert Hendry, Sandia National Laboratories, USA

## MS13

## Uncertainty Quantification in Earth System Modeling, Observation, and Prediction - Part II of III

2:00 PM-4:00 PM

Room: Verelst Room - 2nd Floor

#### For Part 1 see MS5 For Part 3 see MS22

Uncertainty quantification (UQ) for predicting the evolution of the earth system using limited observations for both model development and testing presents challenges to science, mathematics, statistics, and computation. The goal of the minisymposium is to provide a forum for these diverse communities to discuss ideas that will advance confidence in model predictions of the earth system. We are open to any topic that advances this goal including the estimation and representation of low and high dimensional uncertainties in single or multiple earth system components, emulation of physics-based numerical models, and use of new approaches to information theoretic metrics.

Organizer: Guang Lin Pacific Northwest National Laboratory, USA

Organizer: Charles Jackson University of Texas at Austin, USA

Organizer: James Gattiker Los Alamos National Laboratory, USA

2:00-2:25 High Performance Computation of Spatial Field Estimates James Gattiker, Los Alamos National

Laboratory, USA

## 2:30-2:55 Uncertainty Quantification in the Wind-Wave Model WaveWatch-III

Peter Challenor, University of Exeter, United Kingdom; Ben Timmermans and Christine Gommenginger, National Oceanography Centre, United Kingdom

#### 3:00-3:25 Computational Methods for Large Multivariate Spatio-Temporal Computer Model Outputs

Bohai Zhang, Texas A&M University, USA; Alex Konomi, Pacific Northwest National Laboratory, USA; *Huiyan Sang*, Texas A&M University, USA; Guang Lin, Pacific Northwest National Laboratory, USA

#### 3:30-3:55 Simulating and Analyzing Massive Multivariate Remote Sensing Data

*Emily L. Kang*, University of Cincinnati, USA; Hai M. Nguyen, Jet Propulsion Laboratory, California Institute of Technology; Noel Cressie, University of Wollongong, Australia; Amy Braverman and Timothy Stough, Jet Propulsion Laboratory, California Institute of Technology, USA

### Monday, March 31

## MS14 UQ Methods in Lowdimensional Subspaces for Turbulent Dynamical Systems - Part II of III

2:00 PM-4:00 PM

Room: Percival Room - 2nd Floor

#### For Part 1 see MS6 For Part 3 see MS23

Turbulent dynamical systems are characterized by both a large dimensional phase space and a large dimension of instabilities. The existence of these persistent or intermittent instabilities is associated with strong energy transfers between dynamical components that lead to broad energy spectra and strongly non-Guassian statistics. This minisymposium focuses on efficient uncertainty quantification methods designed to provide higher-order statistical information for quantities that 'live' in low-dimensional spaces while they still respect the complex dynamical features connected with the turbulent character of these systems.

Organizer: Themistoklis Sapsis Massachusetts Institute of Technology, USA

Organizer: Andrew Majda Courant Institute of Mathematical Sciences, New York University, USA

#### 2:00-2:25 Sparsity, Sensitivity and Encoding/decoding of Nonlinear Dynamics using Machine Learning Methods

Nathan Kutz and Steven Brunton, University of Washington, USA

#### 2:30-2:55 Statistical Prediction of Extreme Events in Nonlinear Waves William Cousins and Themistoklis Sapsis, Massachusetts Institute of Technology, USA

#### 3:00-3:25 Constrained Orthogonal Decomposition for Reduced Order Modeling of High-Reynolds-number Shear Flows

Maciej Balajewicz, Stanford University, USA

#### 3:30-3:55 Blended Particle Filtering Algorithms for Turbulent Dynamical Systems

*Di Qi*, New York University, USA; Andrew Majda, Courant Institute of Mathematical Sciences, New York University, USA; Themistoklis Sapsis, Massachusetts Institute of Technology, USA

## MS15

## Uncertainty in Environmental Evaluation and Management - Part I of II

2:00 PM-4:00 PM

Room:Savannah Room - Lobby Level

#### For Part 2 see MS32

Scientists must provide regulators with defensible quantification of uncertainties associated with sometimes controversial environmental problems (e.g. sustainability, resources management, climate change and impacts, carbon sequestration, fracking). This sessions explores how conceptual and data uncertainties are represented, evaluated, and reduced; how uncertainty quantification is used in risk analysis, decision support, and law. Of interest are probabilistic and non-probabilistic metrics of judging models against data, ranking alternative models and testing hypotheses; sensitivity analyses for unraveling sources of uncertainty; data collection strategies optimized to reduce uncertainty; and how uncertainty measures inform enforcement strategies and legal frameworks.

Organizer: Mary Hill U.S. Geological Survey, USA

Organizer: Emanuele Borgonovo Bocconi University, Italy

Organizer: Clayton G. Webster Oak Ridge National Laboratory, USA

#### 2:00-2:25 Global Sensitivity Methods: Some Issues and Solutions

*Emanuele Borgonovo*, Bocconi University, Italy

#### 2:30-2:55 Holistic Uncertainty Management for Environmental Decision Support

Anthony J. Jakeman and Joseph H. Guillaume, Australian National University, Australia

#### 3:00-3:25 On the Quantity and Quality of Information Provided by Models and Induction

Grey Nearing, NASA, USA

#### 3:30-3:55 Uncertainty Quantification in the Presence of Subsurface Heterogeneity

Francesca Boso and Daniel M. Tartakovsky, University of California, San Diego, USA

### Monday, March 31

## MS16 UQ Challenge Benchmarks -Part I of II

2:00 PM-4:00 PM

Room: Plimsoll - Lobby Level

#### For Part 2 see MS33

This minisymposium presents new benchmark challenge problems that can serve as a basis for developing, assessing, and improving UQ capabilities. We are proposing a community approach to the challenge of developing appropriate benchmarks. Ideally, a benchmark would be defined as a "progression" or series of problems of increasing complexity, with an ability to refine or redefine the problems as the progression unfolds (over time), based on community input. The benchmark problems presented in this MS are refinements of initial ideas presented at USNCCM12 in July, 2013.

Organizer: James R. Stewart Sandia National Laboratories, USA

Organizer: Roger Ghanem University of Southern California, USA

Organizer: Christian Soize Université Paris-Est, France

#### 2:00-2:25 Uq Challenge Benchmarks Overview

James R. Stewart, Sandia National Laboratories, USA; Roger Ghanem, University of Southern California, USA; Christian Soize, Université Paris-Est, France

#### 2:30-2:55 Uq Benchmark Problems for Multiphysics Modeling

Maarten Arnst, Université de Liège, Belgium

#### 3:00-3:25 Uq Benchmark Problems for Subsurface Flows

Dongxiao Zhang, Peking University, China

#### 3:30-3:55 UQ Benchmark Progression of Turbulent Wall-Bounded Flows

Michael Emory and Francisco Palacios, Stanford University, USA; Paul Constantine, Colorado School of Mines, USA; Gianluca Iaccarino, Stanford University, USA

## CP3 Climate

2:00 PM-4:00 PM

Room: Vernon Room - 2nd Floor

Chair: Pania Newell, Sandia National Laboratories, USA

#### 2:00-2:15 Climate Change and Public Health, Accounting for Uncertainty Between Air Quality and Asthma

Stacey Alexeeff, National Center for Atmospheric Research, USA

#### 2:20-2:35 Multi-Model Ensemble Assimilation for Enhance Model Prediction: Specification of Ionosphere-Thermosphere Environment

Humberto C. Godinez and Michael Shoemaker, Los Alamos National Laboratory, USA; Sean Elvidge, University of Birmingham, United Kingdom; Josef Koller, Los Alamos National Laboratory, USA

#### 2:40-2:55 Uncertainty Qualification in Hurricane Risk Assessment

Shurong Fang and Yue Li, Michigan Technological University, USA

## 3:00-3:15 Two Approaches to Calibration in Metrology

Mark Campanelli, National Renewable Energy Laboratory, USA

#### 3:20-3:35 Sensitivity Analysis of Coupled Flow and Geomechanical Effects on Predictining the Surface Uplift at InSalah

Pania Newell, Hongkyu Yoon, Mario Martinez, and Joseph Bishop, Sandia National Laboratories, USA; Steven Bryant, University of Texas at Austin, USA

#### 3:40-3:55 Quantifying Initial Conditions Uncertainty in Gulf of Mexico Circulation Forecasts Using a Non-Intrusive Polynomial Chaos Method

Mohamed Iskandarani and Matthieu Le Henaff, University of Miami, USA; W. Carlisle Thacker, CIMAS, USA; Omar M. Knio, Duke University, USA; Ashwanth Srinivasan, University of Miami, USA Monday, March 31

## CP4 Algorithms and Software

2:00 PM-4:00 PM

Room:Sloane Room - 2nd Floor

Chair: Ana Maria Soane, Towson University, USA

#### 2:00-2:15 A Multigrid Method for Optimal Control Problems Constrained by Elliptic Equations with Stochastic Diffusion Coefficients

Andrei Draganescu, University of Maryland, Baltimore County, USA

#### 2:20-2:35 Multigrid Preconditioners for Stochastic Optimal Control Problems with Elliptic Spde Constraints

Ana Maria Soane, Towson University, USA

#### 2:40-2:55 Uncertainty Quantification for Robust Optimization: Information Theory and Extended Relational Algebra of Polytopes

Abhilasha Aswal, Anushka Chandrababu, and G. N. Srinivasa Prasanna, International Institute of Information Technology, India

#### 3:00-3:15 Uqlab: An Advanced Software Framework for Uncertainty Quantification

Stefano Marelli and Bruno Sudret, ETH Zürich, Switzerland

#### 3:20-3:35 A New Uncertainty-Bearing Floating-Point Arithmetic

Chengpu Wang, Independent Researcher

#### 3:40-3:55 Hierarchical Preconditioners in the Context of Stochastic Galerkin Finite Elements

Bedrich Sousedik, University of Maryland, USA; Howard C. Elman, University of Maryland, College Park, USA; Roger Ghanem, University of Southern California, USA

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## Coffee Break

4:00 PM-4:30 PM

Room:Regency Foyer and Promenade - 2nd Floor

## Monday, March 31

## **MS17**

## Characterizing Sample Distribution Properties and their Impact on Experimental Design

4:30 PM-6:30 PM

Room:Ballroom A - 2nd Floor

Many times sample distributions for uncertainty quantification are designed for abstract properties such as separation and spatial coverage, and these properties when projected to lower dimensions. In this minisymposium we also consider the (Fourier) spectrum of the points---something that is often overlooked in the UQ community. We consider some directly relevant properties, both on their own and how they depend on spectra. We consider properties of the function being sampled, namely the function or surrogate values at particular points, and their effect on the accuracy (bias) and error (variance) of the estimate of the quantity of interest.

Organizer: Scott A. Mitchell Sandia National Laboratories, USA

Organizer: Mohamed S. Ebeida Sandia National Laboratories, USA

#### 4:30-4:55 Fourier Analysis of Stochastic Sampling Strategies for Assessing Bias and Variance in Integration

*Kartic Subr*, Disney Research UK, The Walt Disney Company, United Kingdom

#### 5:00-5:25 POF-Darts: Geometric Adaptive Sampling for Probability of Failure

Mohamed S. Ebeida, Sandia National Laboratories, USA; *Rui Wang*, University of Massachusetts, USA

#### 5:30-5:55 Exploring High Dimensional Spaces with Hyperplane Sampling

Scott A. Mitchell, Sandia National Laboratories, USA

## 6:00-6:25 Building Surrogate Models with Quantifiable Accuracy

Hany S. Abdel-Khalik and Congjian Wang, North Carolina State University, USA

## MS18

## Numerical Approximation of High-dimensional Stochastic Equations - Part II of IV

4:30 PM-6:30 PM

Room:Ballroom B - 2nd Floor

#### For Part 1 see MS1 For Part 3 see MS34

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 are affected by large amounts of uncertainty. For higher accuracy in computational simulations, approximations must increase the number of random variables (dimensions), and expend more effort resolving smooth or even discontinuous behavior within each individual dimension. The resulting explosion in computational effort is a symptom of the efforts effort is a symptom of curse of dimensionality. This minisymposium aims at exploring efforts related to efficient stochastic Galerkin, collocation and Monte Carlo finite element methods, error analysis, anisotropy and adaptive methods, multi-level and multiresolution analysis, random sampling and sparse grids.

Organizer: Clayton G. Webster Oak Ridge National Laboratory, USA

Organizer: Michael Griebel Universitaet Bonn, Germany

#### 4:30-4:55 A Generalized Stochastic Collocation Approach to Constrained Optimization for Random Data Identification Problems

Max Gunzburger, Florida State University, USA; Clayton G. Webster, Oak Ridge National Laboratory, USA

#### 5:00-5:25 Scalable Algorithms for Design of Experiments on Extreme Scales

Richard Archibald, Oak Ridge National Laboratory, USA

continued in next column

#### 5:30-5:55 Hierarchical Sparse Adaptive Sampling in High Dimension

*Omar M. Knio* and Justin Winokur, Duke University, USA; Olivier P. Le Maitre, LIMSI-CNRS, France

6:00-6:25 Not available at time of publication

Michael Griebel, Universitaet Bonn, Germany

### Monday, March 31

## MS19 Filtering, Data Assimilation, and UQ - Part II of III

4:30 PM-6:30 PM

Room:Ballroom D - 2nd Floor

#### For Part 1 see MS2 For Part 3 see MS27

It is recently becoming amenable to take a probabilistic approach to the solution of inverse problems. Solution of the sequential inverse problem, in which the data arrives online, is known as filtering. This subject has enjoyed a long-standing symbiosis between classical and probabilistic approaches. Data Assimilation can be viewed as a bridge between these, built out of the necessity to get solutions to the filtering problem quickly for very high dimensional problems in atmospheric and oceanographic science. This minisymposium aims to bring together experts interested in filtering, Data Assimilation, and UQ to share their latest ideas and project forward.

Organizer: Kody Law King Abdullah University of Science &Technology (KAUST), Saudi Arabia

Organizer: Raul F. Tempone King Abdullah University of Science & Technology (KAUST), Saudi Arabia

#### 4:30-4:55 Data Assimilation and Noise Modeling

Matthias Morzfeld, Lawrence Berkeley National Laboratory, USA; Alexander J. Chorin, University of California, Berkeley, USA

## 5:00-5:25 Bayesian Data Assimilation with Optimal Transport Maps

Tarek Moselhy, Alessio Spantini, and *Youssef M. Marzouk*, Massachusetts Institute of Technology, USA

#### 5:30-5:55 Pseudo-Orbit Data Assimilation and the Roles of Uncertainty in Multi-Model Forecasting

Lenny Smith, London School of Economics, United Kingdom

#### 6:00-6:25 Reduced Stochastic Forecast Models in Data Assimilation

Georg A. Gottwald, University of Sydney, Australia; *Lewis Mitchell*, University of Vermont, USA; Alberto Carrassi, University of Barcelona, Spain

## MS20 Stochastic Evolution

## Equations and Exit Problems - Part II of II

4:30 PM-6:30 PM

Room:Ballroom E - 2nd Floor

#### For Part 1 see MS11

This minisymposium explores recent work of exit problems that arise in the context of stochastic evolution equations, drawn from application areas ranging from nonlinear optics to fluid dynamics to climate models. The presence of lowdimensional dynamics mitigates the challenge introduced by the absence of a gradient flow in many of these systems. The exits themselves are rare events, suggesting techniques borrowed from large deviation theory.

Organizer: Richard O. Moore New Jersey Institute of Technology, USA

Organizer: Tobias Schaefer City University of New York, Staten Island, USA

#### 4:30-4:55 Models of Large Deviations and Rare Events for Optical Pulses

*William Kath*, Northwestern University, USA; Jinglai Li, Shanghai Jiao Tong University, China

#### 5:00-5:25 Radiation's Role in Simulating Rare Events in Lightwave Systems

Daniel Cargill, Southern Methodist University, USA; Richard O. Moore, New Jersey Institute of Technology, USA; William Kath, Northwestern University, USA

#### 5:30-5:55 Optimal Least Action Control for Manipulating Noisy Network Dynamics

Danny Wells, William Kath, and Adilson E. Motter, Northwestern University, USA

#### 6:00-6:25 Assessing Uncertainty in Mode-Locked Lasers with Feedback

Richard O. Moore, New Jersey Institute of Technology, USA

## Monday, March 31

## MS21 Model Form Uncertainty in

Modeling, Simulation, and Analysis - Part II of III

4:30 PM-6:30 PM

Room:Ballroom F - 2nd Floor

#### For Part 1 see MS12 For Part 3 see MS29

Model form uncertainty is one of the earliest and most important sources of uncertainty in the modeling and simulation process, yet it is the least understood and hardest to quantify, because it is often confounded with other uncertainty sources. This minisymposium intends to focus on state-of-the-art methods to quantify model form uncertainty, including probabilistic and non-probabilistic approaches. A clear understanding of these approaches as to what they quantify and how to integrate the quantification of model form uncertainty with other uncertainty sources will make a significant contribution towards assessing and improving the confidence in simulation-based prediction.

Organizer: Yan Wang Georgia Institute of Technology, USA

Organizer: Sankaran Mahadevan Vanderbilt University, USA

Organizer: Laura Swiler Sandia National Laboratories, USA

#### 4:30-4:55 Quantification of Model Form Uncertainty in Molecular Dynamics Simulation

Yan Wang, David McDowell, Joel Blumer, and Aaron Tallman, Georgia Institute of Technology, USA

#### 5:00-5:25 Addressing Both Parameter and Model Form Uncertainties in Simulation-Based Robust Design

Wei Chen and Dan Apley, Northwestern University, USA

## 5:30-5:55 Interval Model Uncertainty in Nonlinear Fea

Robert Mullen, University of South Carolina, USA; Rafi L. Muhanna, Georgia Institute of Technology, USA

#### 6:00-6:25 Model Discrepancy in Physical System Models

Habib N. Najm, Sandia National Laboratories, USA; Roger Ghanem, University of Southern California, USA; Jaideep Ray and Khachik Sargsyan, Sandia National Laboratories, USA Monday, March 31

## **MS22**

## Uncertainty Quantification in Earth System Modeling, Observation, and Prediction -Part III of III

4:30 PM-6:30 PM

Room: Verelst Room - 2nd Floor

### For Part 2 see MS13

Uncertainty quantification (UQ) for predicting the evolution of the earth system using limited observations for both model development and testing presents challenges to science, mathematics, statistics, and computation. The goal of the minisymposium is to provide a forum for these diverse communities to discuss ideas that will advance confidence in model predictions of the earth system. We are open to any topic that advances this goal including the estimation and representation of low and high dimensional uncertainties in single or multiple earth system components, emulation of physics-based numerical models, and use of new approaches to information theoretic metrics.

Organizer: Guang Lin Pacific Northwest National Laboratory, USA

Organizer: Charles Jackson University of Texas at Austin, USA

Organizer: James Gattiker

## Los Alamos National Laboratory, USA 4:30-4:55 Uncertainty Quantification for

### NASA's Orbiting Carbon Observatory 2 Mission

Amy Braverman and Mike Gunson, Jet Propulsion Laboratory, California Institute of Technology, USA

#### 5:00-5:25 Uncertainty Quantification in Aerosol and Atmospheric Physics

Leighton Regayre, University of Leeds, United Kingdom

#### 5:30-5:55 Exploring a Cloud Microphysics Model Using Statistical Emulation

Jill Johnson, Zhiqiang Cui, Ken Carslaw, and Lindsay Lee, University of Leeds, United Kingdom

#### 6:00-6:25 Calibration and Uq for Test Beds in the Ocean

*K. Sham Bhat*, James Gattiker, and Matthew Hecht, Los Alamos National Laboratory, USA

## MS23

### UQ Methods in Lowdimensional Subspaces for Turbulent Dynamical Systems - Part III of III

## 4:30 PM-6:00 PM

Room: Percival Room - 2nd Floor

#### For Part 2 see MS14

Turbulent dynamical systems are characterized by both a large dimensional phase space and a large dimension of instabilities. The existence of these persistent or intermittent instabilities is associated with strong energy transfers between dynamical components that lead to broad energy spectra and strongly non-Guassian statistics. This minisymposium focuses on efficient uncertainty quantification methods designed to provide higher-order statistical information for quantities that 'live' in low-dimensional spaces while they still respect the complex dynamical features connected with the turbulent character of these systems.

Organizer: Themistoklis Sapsis Massachusetts Institute of Technology, USA

Organizer: Andrew Majda Courant Institute of Mathematical Sciences, New York University, USA

#### 4:30-4:55 Closed-Loop Turbulence Control - A Systematic Strategy for the Nonlinearities

Bernd R. Noack, Thomas Duriez, Vladimir Parezanovic, Jean-Charles Laurentie, Michael Schlegel, Eurika Kaiser, and Laurent Cordier, CNRS, France; Andreas Spohn, ENS, France; Jean-Paul Bonnet, CNRS, France; Marek Morzynski, Poznan University of Technology, Poland; Marc Segond and Markus W Abel, Ambrosys GmbH, Germany; Steven Brunton, University of Washington, USA

#### 5:00-5:25 Model Reduction for Stochastic Fluid Flows Using Dynamically Orthogonal and Bi-Orthogonal Methods

Minseok Choi, Brown University, USA

#### 5:30-5:55 Mechanisms of Derivative-Based Uncertainty and Sensitivity Propagation in Barotropic Ocean Models

Alex Kalmikov, Massachusetts Institute of Technology, USA

### Monday, March 31

## MS24 UQ and Environmental Statistics

4:30 PM-6:30 PM

Room:Savannah Room - Lobby Level

The environmental sciences often use data that are derived from complex climate models and require development of advanced statistical methods for proper analysis. This session will address these issues from a UQ and statistical perspective. The talks will cover how to use high-dimensional observational data sets to quantify uncertainty in climate model parameters; evaluating uncertainty in satellite data to improve understanding of the role of salinity in ocean circulation; combining data using hierarchical modeling to evaluate anthropogenic influences in extreme weather events; and a new spatial extremes model for the study of precipitation extremes from regional climate models.

Organizer: Jessi Cisewski Carnegie Mellon University, USA

#### 4:30-4:55 Combining High-Dimensional Data from Climate Models and Observations to Sharpen Predictions About Future Climate

Murali Haran, Won Chang, Roman Olson, and Klaus Keller, Pennsylvania State University, USA

#### 5:00-5:25 Spatial Temporal Uncertainty Quantification Methods for Satellite Output

*Elizabeth Mannshardt* and Montserrat Fuentes, North Carolina State University, USA; Frederick Bingham, University of North Carolina, Wilmington, USA

#### 5:30-5:55 Influence of Climate Change on Extreme Weather Events

*Richard Smith*, Statistical and Applied Mathematical Sciences Institute, USA

#### 6:00-6:25 Inference for Hidden Regular Variation in Multivariate Extremes

*Grant B. Weller*, Carnegie Mellon University, USA; Dan Cooley, Colorado State University, USA

### Monday, March 31

## MS25 Large-scale Experimental Analysis - Part II of II

4:30 PM-6:30 PM

Room:Plimsoll - Lobby Level

#### For Part 1 see MS8

The traditional methods for design and analysis of experiments are tooled for circumstances where few explanatory variables are available and few observations are possible. Today, these assumptions are often violated in experiments conducted for uncertainty quantification. Examples include scenarios where data are taken from multiple sources, many predictors need to be studied, or the response is very intricate. Many techniques designed under the limited information paradigm are computationally inefficient or even intractable in these data-rich environments. This minisymposium invites contributions that study experimental design and analysis when large numbers of predictors and/or observations are present.

Organizer: Matthew Plumlee Georgia Institute of Technology, USA

Organizer: Peter Qian University of Wisconsin, Madison, USA

4:30-4:55 Performance Modeling and Optimization in Numerical Simulations

Weichung Wang, National Taiwan University, Taiwan; Ray-Bing Chen, National Cheng Kung University, Taiwan

#### 5:00-5:25 Efficient Inference Using Sparse Grid Experimental Designs

Matthew Plumlee, Georgia Institute of Technology, USA

#### 5:30-5:55 Compressive Sensing for Computational Materials Science Experiments

Shane Reese, Brigham Young University, USA

#### 6:00-6:25 Gaussian Process Adaptive Importance Sampling (GPAIS)

Keith Dalbey and Laura Swiler, Sandia National Laboratories, USA

## CP5 Applications I

4:30 PM-6:10 PM

Room: Vernon Room - 2nd Floor

#### 4:30-4:45 Efficiency of Monte Carlo Parameter Sensitivity Estimators for Chemical Kinetics

*Ting Wang* and Muruhan Rathinam, University of Maryland, Baltimore County, USA

#### 4:50-5:05 *L*<sub>2</sub>-Boosting on Generalized Hoeffding Decomposition for Dependent Variables - Application to Sensitivity Analysis

Magali Champion, Institut de Mathématiques de Toulouse, France; Gaelle Chastaing, Universite Joseph Fourier, France; Sébastien Gadat, Institut de Mathématiques de Toulouse, France; Clémentine Prieur, Universite Joseph Fourier, France

#### 5:10-5:25 New Sensitivity Analysis Subordinated to a Contrast

*Thierry Klein*, Universite de Toulouse, France; Jean-Claude Fort, Université Paris Descartes, France; Nabil Rachdi, EADS Innovation Works, France

#### 5:30-5:45 Morris Screening Combined with Gaussian Process-Based Joint Metamodels for the Sensitivity Analysis of Simulation Codes

Amandine Marrel, Nathalie Marie, and Nadia Perot, CEA, France

#### 5:50-6:05 Experience with Selected Methods for Sensitivity Analysis of a Computational Model with Quasi-Discrete Behavior

Sabine M. Spiessl and Dirk-Alexander Becker, Gesellschaft für Anlagen- und Reaktorsicherheit mbH, Germany

#### Monday, March 31

## CP6 Algorithms I

4:30 PM-6:30 PM

Room:Sloane Room - 2nd Floor

Chair: Joshua G. Mullins, Vanderbilt University, USA

#### 4:30-4:45 Algebraic Quadrature for Uncertainty Quantification

*Henry Wynn* and Jordan Ko, London School of Economics, United Kingdom

#### 4:50-5:05 Uncertainty Quantification in Mesoscopic Modeling and Simulation

*Huan Lei*, Pacific Northwest National Laboratory, USA; Xiu Yang and George E. Karniadakis, Brown University, USA

#### 5:10-5:25 Resource Allocation for Uncertainty Quantification and Reduction

Joshua G. Mullins and Sankaran Mahadevan, Vanderbilt University, USA

#### 5:30-5:45 Quantification of Aleatory and Epistemic Uncertainties in Reliability Assessment

Saideep Nannapaneni and Sankaran Mahadevan, Vanderbilt University, USA; Shankar Sankararaman, NASA Ames Research Center, USA

#### 5:50-6:05 Stochastic Polynomial Interpolation for Uncertainty Quantification with Computer Experiments

Matthias H. Tan, City University of Hong Kong, Hong Kong

#### 6:10-6:25 Analysis for the Least Square Approach with Applications for Uncertainty Quantification

*Tao Zhou* and Zhiqiang Xu, Chinese Academy of Sciences, China; Akil Narayan, University of Massachusetts, Dartmouth, USA

## Dinner Break

6:30 PM-8:00 PM

Attendees on their own

### Monday, March 31

## PP1

## Poster Session

8:00 PM-10:00 PM

Room: Harborside East - River Street Level

Fuzzy Solution of Interval Linear Programming with Fuzzy Constraints Ibraheem Alolyan, King Saud University, Saudia Arabia

#### Multilevel Monte Carlo Simulation for Stochastic Models in Chemical Kinetics

Zane Colgin and Abdul Khaliq, Middle Tennessee State University, USA

#### Sensitivity Analysis of Models with Dynamic Inputs\\ Application to the Impact of the Weather Data on the Performance of Passive Houses

*Floriane Collin*, University of Lorraine, France; Thierry Mara, University of La Réunion, France; Lilianne Denis-Vidal, University of Technology of Compiègne, France; Jeanne Goffart, University of Savoy, France

#### An Adaptive Change Point Based Prediction Model: Application to Transportation Networks

*Gurcan Comert*, Anton Bezuglov, and Sajan Shrestha, Benedict College, USA; Charles Taylor, Norfolk State University, USA

## Analysis of Some Arrival Distributions for Queue Length Estimation Problem

*Gurcan Comert*, April Chappell, and Tia Herring, Benedict College, USA

#### Evaluation of Some Estimators for Arrival Rate and Probe Proportion in Queue Length Estimation Problem

*Gurcan Comert*, Anton Bezuglov, Kenneth Yeadon, and Tatyanna Taylor, Benedict College, USA

#### Uncertainty Quantification for Airfoil Icing Using Polynomial Chaos Expansions

Anthony Degennaro, Clancy Rowley, and Luigi Martinelli, Princeton University, USA

#### A Fractal Model of Time

Jorge Diaz-Castro, University of Puerto Rico, Puerto Rico

#### A Scalable, Adaptive, Hessian-Based Gaussian Mixture Proposal for Large-Scale Statistical Inverse Problems, with Applications to Subsurface Flow

*H. Pearl Flath*, University of Texas at Austin, USA

#### Impacts of Greenland Surface Mass Balance Uncertainties on Ice Sheet Initialization and Predictions of Sea Level Rise in 2100

Gail Gutowski and Charles Jackson, University of Texas at Austin, USA

#### Adapting Actuated Traffic Signal Control Settings with Queue Lengths from Probe Vehicles

Gurcan Comert and *Gary Knight*, Benedict College, USA

Uq of Computational Fluid Dynamics Models in Nuclear Applications Jordan Ko, AREVA Nuclear Power, France

## Uncertainties Propagation and Estimation of a Quantile

*Tatiana Labopin-Richard*, Gamboa Fabrice, and Garivier Aurelien, Institut de Mathématiques de Toulouse, France

#### Matrix-Free Geostatistical Inversion with An Application in Large-Scale Hydraulic Tomography

Jonghyun Lee, Stanford University, USA; Peter K Kitanidis, Stanford University, USA

#### Symmetry in Quantum Turbulence

*Cassandra Oduola*, Texas Southern University, USA; Jaques Richard, Texas A&M University, USA; Christpher Tymczak and Daniel Vrinceanu, Texas Southern University, USA

#### Balanced Split-Step Methods for Stiff Multiscale Stochastic Systems with Uncertainties

*Viktor Reshniak* and Abdul Khaliq, Middle Tennessee State University, USA; David A. Voss, Western Illinois University, USA

### Using Emulators and Hierarchical Models for UQ in Hazard Forecasting

*Regis Rutarindwa* and Elaine Spiller, Marquette University, USA

#### Applications of Statistical Inference in the Design of High-Performance Optical Metamaterials

Niket Thakkar, Randall LeVeque, and David Masiello, University of Washington, USA

#### Regularized Collocation for Spherical Harmonics Gravitational Field Modeling

Pavlo Tkachenko, Sergei Pereverzev, and Valeriya Naumova, RICAM, Austrian Academy of Sciences, Austria

## Tuesday, April 1

Registration 7:30 AM-5:00 PM Room:Registration Booth - 2nd Floor

### Remarks

8:10 AM-8:15 AM Room:Ballroom A/B/C - 2nd Floor

## IP3

# Uncertainty Quantification in Bayesian Inversion

8:15 AM-9:00 AM

Room:Ballroom A/B/C - 2nd Floor Chair: Julia Charrier, Aix-Marseille Université, France

Many problems in the physical sciences require the determination of an unknown field from a finite set of indirect measurements. Examples include oceanography, oil recovery, water resource management and weather forecasting. The Bayesian approach to these problems provides a natural way to provide estimates of the unknown field, together with a quantification of the uncertainty associated with the estimate. In this talk I will describe an emerging mathematical framework for these problems, explaining the resulting well-posedness and stability theory, and showing how it leads to novel computational algorithms. This session was designed to complement MS27.

Andrew Stuart University of Warwick, United Kingdom

## Coffee Break

9:00 AM-9:30 AM



Room:Regency Foyer and Promenade - 2nd Floor

## Tuesday, April 1

## MT3

## Reduced Order Methods for Modelling and Computational Reduction in UQ Problems

9:30 AM-11:30 AM

Room:Ballroom A - 2nd Floor

Chair: Gianluigi Rozza, SISSA, International School for Advanced Studies, Trieste, Italy

We present the state of the art of some reduced order methods for modelling and computational reduction, adapted and developed for uncertainty quantification problems. We first focus on forward problems, then we deal with inverse problems, in particular with optimal control problems. Proper adaptation of reduced basis method and related techniques is introduced. A special attention is devoted to robust optimization under uncertainty. This session is designed to complement MS45.

*Gianluigi Rozza*, SISSA, International School for Advanced Studies, Trieste, Italy; Peng Chen, École Polytechnique Fédérale de Lausanne, Switzerland Tuesday, April 1

## **MS26**

## Advances in Markov Chain Monte Carlo Methods for Large-scale Inverse Problems - Part II of II

### 9:30 AM-11:30 AM

Room:Ballroom B - 2nd Floor

#### For Part 1 see MS9

Inverse problems convert indirect measurements into characterizations of parameters of a system. Parameters are typically related to measurements by a system of PDEs, which are expensive to evaluate. Data are often limited and noisy while the unknown parameters of interest are often high dimensional, or infinite dimensional in principle. Solution of the inverse problem can be cast in a Bayesian setting and thus naturally tackled with Markov chain Monte Carlo (MCMC) methods. However, designing scalable and efficient MCMC methods for high dimensional inverse problems poses a significant challenge. This minisymposium presents recent advances in MCMC methods for solving large-scale inverse problems.

Organizer: Tiangang Cui Massachusetts Institute of Technology, USA

Organizer: Kody Law King Abdullah University of Science &Technology (KAUST), Saudi Arabia

Organizer: Youssef M. Marzouk Massachusetts Institute of Technology, USA

#### 9:30-9:55 Dimension-independent Likelihood-informed MCMC Samplers

*Tiangang Cui*, Massachusetts Institute of Technology, USA; Kody Law, King Abdullah University of Science & Technology (KAUST), Saudi Arabia; Youssef M. Marzouk, Massachusetts Institute of Technology, USA

#### 10:00-10:25 Bayesian Uncertainty Quantification for Differential Equations

Oksana A. Chkrebtii and Dave A. Campbell, Simon Fraser University, Canada; *Mark Girolami* and Ben Calderhead, University College London, United Kingdom

#### 10:30-10:55 A Randomized Map Algorithm for Large-Scale Bayesian Inverse Problems

*Tan Bui-Thanh*, Omar Ghattas, Alen Alexanderian, Noemi Petra, and Georg Stadler, University of Texas at Austin, USA

#### 11:00-11:25 Exploiting Geometry in MCMC Using Optimal Transport Theory

Matthew Parno and Youssef M. Marzouk, Massachusetts Institute of Technology, USA

### Tuesday, April 1

## MS27 Filtering, Data Assimilation, and UQ - Part III of III

9:30 AM-11:30 AM

Room:Ballroom D - 2nd Floor

#### For Part 2 see MS19

It is recently becoming amenable to take a probabilistic approach to the solution of inverse problems. Solution of the sequential inverse problem, in which the data arrives online, is known as filtering. This subject has enjoyed a long-standing symbiosis between classical and probabilistic approaches. Data Assimilation can be viewed as a bridge between these, built out of the necessity to get solutions to the filtering problem quickly for very high dimensional problems in atmospheric and oceanographic science. This minisymposium aims to bring together experts interested in filtering, Data Assimilation, and UQ to share their latest ideas and project forward. This session is designed to complement IP3.

Organizer: Kody Law King Abdullah University of Science &Technology (KAUST), Saudi Arabia

Organizer: Raul F. Tempone King Abdullah University of Science & Technology (KAUST), Saudi Arabia

#### 9:30-9:55 Accuracy of the Optimal Filter for Partially Observed Chaotic Dynamics

Andrew Stuart, and *Daniel Sanz-Alonso*, University of Warwick, United Kingdom

#### 10:00-10:25 Stabilized Low-memory Kalman Filter for High Dimensional Data Assimilation

Heikki Haario and *Alexander Bibov*, Lappeenranta University of Technology, Finland

#### 10:30-10:55 Combined Parameter and State Estimation in Lagrangian Data Assimilation

Naratip Santitissadeekorn, University of North Carolina at Chapel Hill, USA; Christopher Jones, University of North Carolina at Chapel Hill and University of Warwick, United Kingdom

#### 11:00-11:25 Filter Divergence and Enkf

David Kelly, University of Warwick, United Kingdom; Kody Law, King Abdullah University of Science & Technology (KAUST), Saudi Arabia; Andrew Stuart, University of Warwick, United Kingdom

#### Tuesday, April 1

## **MS28**

### Uncertainty Quantification in Fluid Dynamics and Particle Accelerator Physics - Part I of II

9:30 AM-11:30 AM

#### Room:Ballroom E - 2nd Floor

#### For Part 2 see MS36

Uncertainty quantification for simulations is a critical issue, as the models often constitute a primary source of uncertainty. We see how the specific requirements of diverse applications set the framework for justifying and assessing UQ methods. We will present and discuss the efforts to study UQ in many realistic applications from the design of particle accelerators to fusion energy to astrophysics to turbulent combustion.

Organizer: Tulin Kaman ETH Zürich and Paul Scherrer Institute, Switzerland

Organizer: James G. Glimm State University of New York, Stony Brook, USA

#### 9:30-9:55 V&V and Uncertainty Quantification for Turbulent Mixing in Inertial Confinement Fusion Capsules

James G. Glimm, Jeremy Melvin, Verinder Rana, and Hyunkyung Lim, State University of New York, Stony Brook, USA; Baolian Cheng, Los Alamos National Laboratory, USA

#### 10:00-10:25 Quantification of Multiple and Disparate Uncertainties in the HyShot II Scramjet

Johan Larsson, University of Maryland, USA; Michael Emory, Stanford University, USA; Paul Constantine, Colorado School of Mines, USA; Gianluca Iaccarino, Stanford University, USA

#### 10:30-10:55 Uncertainty Quantification of Transient Turbulent Flows Using Dynamical Orthogonality Themistoklis Sapsis, Massachusetts Institute

of Technology, USA

#### 11:00-11:25 Uncertainty Quantification in Astrophysical Simulations of White Dwarf Stars

Alan Calder, Max Katz, and Douglas Swesty, Stony Brook University, USA; Grace Zhang, Ward Melville High School, USA

### Tuesday, April 1

## MS29

## Model Form Uncertainty in Modeling, Simulation, and Analysis - Part III of III

9:30 AM-11:30 AM

Room:Ballroom F - 2nd Floor

#### For Part 2 see MS21

Model form uncertainty is one of the earliest and most important sources of uncertainty in the modeling and simulation process, yet it is the least understood and hardest to quantify, because it is often confounded with other uncertainty sources. This minisymposium intends to focus on state-of-the-art methods to quantify model form uncertainty, including probabilistic and non-probabilistic approaches. A clear understanding of these approaches as to what they quantify and how to integrate the quantification of model form uncertainty with other uncertainty sources will make a significant contribution towards assessing and improving the confidence in simulation-based prediction.

Organizer: Yan Wang Georgia Institute of Technology, USA

Organizer: Sankaran Mahadevan Vanderbilt University, USA

Organizer: Laura Swiler Sandia National Laboratories, USA

#### 9:30-9:55 Estimation of Structural Error in the Community Land Model Using Latent Heat Observations

Jaideep Ray, Sandia National Laboratories, USA; Maoyi Huang and Zhangshuan Hou, Pacific Northwest National Laboratory, USA; Laura Swiler, Sandia National Laboratories, USA

#### 10:00-10:25 Representing Model Form Uncertainty: A Case Study in Chemical Kinetics

*Rebecca Morrison*, Robert D. Moser, Todd Oliver, and Chris Simmons, University of Texas at Austin, USA

continued on next page

Tuesday, April 1

## **MS29**

## Model Form Uncertainty in Modeling, Simulation, and Analysis - Part III of III

9:30 AM-11:30 AM

Room:Ballroom F - 2nd Floor continued

#### 10:30-10:55 Probabilistic Representations of Model Inadequacy for RANS Turbulence Models

*Todd Oliver* and Robert D. Moser, University of Texas at Austin, USA

#### 11:00-11:25 Quantification of Model-Form Uncertainty in Turbulence Mixing Models

Gianluca Iaccarino and Michael Emory, Stanford University, USA; *Catherine Gorle*, University of Antwerp, Belgium

#### Tuesday, April 1

## MS30

## Controlling Uncertainty in PDE-Constrained Optimization

9:30 AM-11:30 AM

Room: Verelst Room - 2nd Floor

Optimization problems governed by PDEs arise in numerous science and engineering applications. In many application problems, PDE parameters and coefficients are estimated from noisy, empirical data. Such estimation injects uncertainty into the optimization problem. It is essential to determine reliable and robust optimal solutions in order to control uncertainty in the optimized system. This minisymposium presents novel problem formulations and solution techniques for the robust and risk-averse solution to PDEconstrained optimization problems under uncertainty.

Organizer: Drew P. Kouri Sandia National Laboratories, USA

Organizer: Denis Ridzal Sandia National Laboratories, USA

Organizer: Bart G. Van Bloemen Waanders

Sandia National Laboratories, USA

#### 9:30-9:55 Sparse-grid Algorithms for PDE-constrained Optimization Under Uncertainty

Bart G. Van Bloemen Waanders, Denis Ridzal, and Drew P. Kouri, Sandia National Laboratories, USA

#### 10:00-10:25 Multilevel and Adaptive Methods for Risk-Averse PDE-Constrained Optimization

Drew P. Kouri, Sandia National Laboratories, USA

#### 10:30-10:55 Topology Optimization for Nano and Macro-Scale Lithography Processes with Uncertainties

Boyan S. Lazarov, Mingdong Zhou, and Ole Sigmund, Technical University of Denmark, Denmark

## 11:00-11:25 Stochastic Optimization of Gas Networks

Victor Zavala and *Naiyuan Chiang*, Argonne National Laboratory, USA

### Tuesday, April 1

## **MS31**

## Low-rank and Sparse Representation Methods for Uncertainty Quantification -Part I of III

9:30 AM-11:30 AM

Room:Percival Room - 2nd Floor

### For Part 2 see MS39

Approximations of stochastic equations may lead to extremely high dimensional problems, which may be handled by adaptive low-rank/sparse representations. These may also be applied to statistical inverse problems of parameter identification. In addition, the solution of the forward and inverse problems can be considered as a whole adaptive process controlled by error estimators. The aim of this minisymposium is to bring together experts in adaptive methods for the discretisation and the solution of stochastic/multiparametric forward and inverse problems, and experts in lowrank/sparse tensor methods. This includes Bayesian methods, control procedures, and algorithms such as "design of experiments."

Organizer: Martin Eigel WIAS, Berlin, Germany

Organizer: Loïc Giraldi Ecole Centrale de Nantes, France

Organizer: Alexander Litvinenko King Abdullah University of Science &Technology (KAUST), Saudi Arabia

Organizer: Hermann Matthies Technische Universität Braunschweig, Germany

Organizer: Anthony Nouy Ecole Centrale de Nantes, France

## 9:30-9:55 Nonlinear Bayesian Updates and Low-Rank Approximations

Hermann Matthies, Technische Universität Braunschweig, Germany; Alexander Litvinenko, King Abdullah University of Science & Technology (KAUST), Saudi Arabia; Oliver Pajonk, SPT Group GmbH, Germany; Bojana Rosic, TU Braunschweig, Germany

#### 10:00-10:25 Regularising Ensemble Kalman Methods for Inverse Problems

Marco Iglesias, University of Nottingham, United Kingdom

#### 10:30-10:55 Optimal Design of Experiments: a Sparse-Integration Perspective

Wolfgang Nowak, University of Stuttgart, Germany

#### 11:00-11:25 Advances in Adaptive Stochastic Galerkin FEM

Martin Eigel, WIAS, Berlin, Germany; Claude J. Gittelson, Purdue University, USA; Christoph Schwab, ETH Zürich, Switzerland; Elmar Zander, Technical University Braunschweig, Germany Tuesday, April 1

## **MS32**

Uncertainty in Environmental Evaluation and Management - Part II of II

## 9:30 AM-11:30 AM

Room:Savannah Room - Lobby Level

#### For Part 1 see MS15

Scientists must provide regulators with defensible quantification of uncertainties associated with sometimes controversial environmental problems (e.g. sustainability, resources management, climate change and impacts, carbon sequestration, fracking). This sessions explores how conceptual and data uncertainties are represented, evaluated, and reduced; how uncertainty quantification is used in risk analysis, decision support, and law. Of interest are probabilistic and non-probabilistic metrics of judging models against data, ranking alternative models and testing hypotheses; sensitivity analyses for unraveling sources of uncertainty; data collection strategies optimized to reduce uncertainty; and how uncertainty measures inform enforcement strategies and legal frameworks.

Organizer: Mary Hill U.S. Geological Survey, USA

Organizer: Emanuele Borgonovo Bocconi University, Italy

Organizer: Clayton G. Webster Oak Ridge National Laboratory, USA

#### 9:30-9:55 Exploring How Parameter Importance to Prediction Changes in Parameter Space

Olda Rakovec, University of Wageningen, Netherlands; *Mary Hill*, U.S. Geological Survey, USA; Martyn Clark, University of Colorado Boulder, USA

#### 10:00-10:25 Using Airborne Geophysical Data to Reduce Groundwater Model Uncertainty

Burke J. Minsley, U.S. Geological Survey, USA; Nikolaj Christensen and Steen Christensen, Aarhus University, Denmark

#### 10:30-10:55 A Bayesian Framework for Uncertainty Quantification with Application to Groundwater Reactive Transport Modeling

Ming Ye, Florida State University, USA

#### 11:00-11:25 Assessment of Predictive Performance of Bayesian Model Averaging in Reactive Transport Models

Dan Lu and Ming Ye, Florida State University, USA; Gary Curtis, U.S. Geological Survey, USA Tuesday, April 1

## MS33 UQ Challenge Benchmarks - Part II of II

#### 9:30 AM-11:00 AM

Room: Plimsoll - Lobby Level

#### For Part 1 see MS16

This minisymposium presents new benchmark challenge problems that can serve as a basis for developing, assessing, and improving UQ capabilities. We are proposing a community approach to the challenge of developing appropriate benchmarks. Ideally, a benchmark would be defined as a "progression" or series of problems of increasing complexity, with an ability to refine or redefine the problems as the progression unfolds (over time), based on community input. The benchmark problems presented in this MS are refinements of initial ideas presented at USNCCM12 in July, 2013.

Organizer: James R. Stewart Sandia National Laboratories, USA

Organizer: Roger Ghanem University of Southern California, USA

Organizer: Christian Soize Université Paris-Est, France

#### 9:30-9:55 Validating Extrapolative Predictions: Benchmark Problems and Research Issues

Robert D. Moser, Todd Oliver, Damon McDougall, and Chris Simmons, University of Texas at Austin, USA

#### 10:00-10:25 Benchmark Problems for Predictive Material Behavior, Part 1

Roger Ghanem, University of Southern California, USA

#### 10:30-10:55 Benchmark Problems for Predictive Material Behavior, Part 2

Somnath Ghosh, Johns Hopkins University, USA

#### Tuesday, April 1

## CP7 Multilevel Methods 9:30 AM-11:30 AM

Room: Vernon Room - 2nd Floor

Chair: Daniel Elfverson, Uppsala University, Sweden

#### 9:30-9:45 Multilevel Monte Carlo Methods for Rare Event Probabilities and Quantiles

Daniel Elfverson, Fredrik Hellman, and Axel Målqvist, Uppsala University, Sweden

#### 9:50-10:05 Optimization of Mesh Hierarchies for Multilevel Monte Carlo

Abdul Lateef Haji Ali and Nathan Collier, King Abdullah University of Science & Technology (KAUST), Saudi Arabia; Fabio Nobile and Erik Schwerin, EPFL, France; Raul F. Tempone, King Abdullah University of Science & Technology (KAUST), Saudi Arabia

#### 10:10-10:25 Multilevel Monte Carlo Methods with Control Variate for Elliptic SPDEs

*Francesco Tesei*, École Polytechnique Fédérale de Lausanne, Switzerland; Fabio Nobile, EPFL, France

#### 10:30-10:45 Multilevel Monte Carlo Simulations with Algebraically Constructed Coarse Spaces

*Umberto E. Villa* and Panayot Vassilevski, Lawrence Livermore National Laboratory, USA

#### 10:50-11:05 Multilevel MCMC/SMC Sampling for Inverse Electromagnetic Scattering

*Pierre Minvielle-Larrousse*, CEA/CESTA, France; Adrien Todeschini, Francois Caron, and Pierre Del Moral, INRIA, France

#### 11:10-11:25 Estimation of Multi-Level Extrapolation Confidence

Chenzhao Li and Sankaran Mahadevan, Vanderbilt University, USA Tuesday, April 1

## CP8 Applications II 9:30 AM-11:10 AM

Room:Sloane Room - 2nd Floor

Chair: Christopher W. Miller, US Naval Research Laboratory, USA

#### 9:30-9:45 Uncertainty Quantification in Nanowire Sensors Using the Stochastic Nonlinear Poisson-Boltzmann Equation

Clemens F. Heitzinger, Arizona State University, USA and Vienna University of Technology, Austria; Amirreza Khodadadian, Vienna University of Technology, Austria

#### 9:50-10:05 Dissipative 2D Structures in Quintic Ginzburg Landau Equation

Harihar Khanal and Stefan C. Mancas, Embry-Riddle Aeronautical University, USA

#### 10:10-10:25 The Effects of Design Uncertainties on Multiple Order Step Etalon Spectrometers

*Christopher W. Miller* and Michael Yetzbacher, US Naval Research Laboratory, USA

#### 10:30-10:45 First Order *k*-th Moment Analysis for the Nonlinear Eddy Current Problem

*Ulrich Roemer*, Sebastian Schöps, and Thomas Weiland, Technische Universitaet Darmstadt, Germany

#### 10:50-11:05 Searching Chemical Spectroscopy Libraries

*William E. Wallace* and Anthony Kearsley, National Institute of Standards and Technology, USA

## Lunch Break

11:30 AM-1:00 PM

Attendees on their own
### PD1 Funding Agency Panel Discussion

11:45 AM-12:45 PM

Room:Ballroom A/B/C - 2nd Floor

Chair: Philip Stark, University of California, Berkeley, USA

Chair: Marcia McNutt, Science Magazine, American Association for the Advancement of Science, USA

Representatives from three US funding agencies and one German funding agency will give short presentations about the opportunities available within their agencies for supporting UQ-related research. Given the international makeup of the participants and given the geophysics applications theme of the conference, the participants will also speak about opportunities within their agencies for supporting international and interdisciplinary research collaborations. Some time will also be reserved for questions from the audience.

### Fariba Fahroo

Air Force Office of Scientific Research, USA

### Frank Kiefer

DFG (German Research Foundation), Germany

### Steve Lee

U.S. Department of Energy, USA

### Junping Wang

National Science Foundation, USA

Tuesday, April 1

## IP4

## Evidence-based Treatment of Computer Experiments

1:00 PM-1:45 PM

Room:Ballroom A/B/C - 2nd Floor

Chair: Philip Stark, University of California, Berkeley, USA

Using a complex computer model for optimization, sensitivity analysis, etc. typically requires a surrogate (approximation) to enable many (fast) predictions. Building a surrogate is done via a set of runs at designated inputs that is, a computer experiment. Choices must be made to design the experiment and build the surrogate: Design -- How many runs? At what inputs? Methods for Surrogate Building -- Polynomial chaos (PC)? Gaussian process Bayesian methods (GP)? Specifics of Methods -- Which PC? Which GP? Faced with a myriad of competing answers what's a modeler to do? Does it matter? The talk, based on work with John Jakeman, Jason Loeppky and William Welch, will describe an evidence-based approach to compare and evaluate competing methods leading to recommendations and findings, some at variance with common beliefs.

### Jerome Sacks

National Institute of Statistical Sciences, USA

### Intermission

1:45 PM-2:00 PM

### Tuesday, April 1

## MT4 VV&EQ and Reproducible Computational Science

2:00 PM-4:00 PM

Room:Ballroom A - 2nd Floor Chair: Victoria Stodden, Columbia University, USA

This minitutorial will outline relationships between Validation and Verification as understood in the scientific computing community, and Reproducibility as understood across the computational sciences. It will also address notions of inherent uncertainty and sources of error when reproducing computational findings, and trace these back to the established concept of uncertainty quantification. This session is designed to complement MS42.

Victoria Stodden, Columbia University, USA

# MS34

### Numerical Approximation of High-dimensional Stochastic Equations - Part III of IV

2:00 PM-4:00 PM

Room:Ballroom B - 2nd Floor

### For Part 2 see MS18 For Part 4 see MS43

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 are affected by large amounts of uncertainty. For higher accuracy in computational simulations, approximations must increase the number of random variables (dimensions), and expend more effort resolving smooth or even discontinuous behavior within each individual dimension. The resulting explosion in computational effort is a symptom of the efforts effort is a symptom of curse of dimensionality. This minisymposium aims at exploring efforts related to efficient stochastic Galerkin, collocation and Monte Carlo finite element methods, error analysis, anisotropy and adaptive methods, multilevel and multi-resolution analysis, random sampling and sparse grids.

Organizer: Clayton G. Webster Oak Ridge National Laboratory, USA

Organizer: Michael Griebel Universitaet Bonn, Germany

### 2:00-2:25 A Hyperspherical Method for Discontinuity Detection

John Burkardt, Florida State University, USA; Clayton G. Webster and Guannan Zhang, Oak Ridge National Laboratory, USA

### 2:30-2:55 Stochastic Collocation on Arbitrary Nodes via Interpolation

*Dongbin Xiu*, University of Utah, USA; Akil Narayan, University of Massachusetts, Dartmouth, USA

#### 3:00-3:25 A Hierarchical, Multilevel Stochastic Collocation Method for Adaptive Acceleration of PDEs with Random Input Data

*Guannan Zhang* and Clayton G. Webster, Oak Ridge National Laboratory, USA

#### **3:30-3:55 Sparsity in Bayesian Inversion** *Claudia Schillings* and Christoph Schwab,

ETH Zürich, Switzerland

Tuesday, April 1

## **MS35**

### Adaptive Methods in Uncertainty Quantification -Part I of II

2:00 PM-4:00 PM

Room:Ballroom D - 2nd Floor

### For Part 2 see MS44

The computational demand of single simulation runs poses limits to the quantification of uncertainties, especially with non-intrusive methods that aim to approximate the response surface for the problem at hand. Numerical approximations suffer from the curse of dimensionality, and most problems demand high resolution only in certain parameter ranges. To reduce the computational demand, an adaptive representation and exploration of such response surfaces is required. Typical applications encounter non-smooth parameter dependencies or even shock phenomena, such as when measuring leakage at a fault in a cap rock for subsurface flows. This minisymposium addresses the current state of the art of adaptive approaches for non-intrusive methods in uncertainty quantification.

Organizer: Dirk Pflüger Universität Stuttgart, Germany

Organizer: John D. Jakeman Sandia National Laboratories, USA

Organizer: Tobias Neckel *TU München, Germany* 

#### 2:00-2:25 Adaptive Sparse Grid Interpolation Using One-Dimensional Leja Sequences

John D. Jakeman, Sandia National Laboratories, USA; Akil Narayan, University of Massachusetts, Dartmouth, USA

#### 2:30-2:55 Constructing Adaptive and Unstructured Design Samples in Multivariate Space Using Leja Sequences

Akil Narayan, University of Massachusetts, Dartmouth, USA; Dongbin Xiu, University of Utah, USA; John D. Jakeman, Sandia National Laboratories, USA

continued in next column

### 3:00-3:25 Adaptive Sampling for Bayesian Updating with Non-Intrusive Polynomial Chaos Expansions

*Michael Sinsbeck* and Wolfgang Nowak, University of Stuttgart, Germany

### 3:30-3:55 Kernel-Based Adaptive Methods in Large-Scale Cfd Problems with Uncertainties

Peter Zaspel, Universität Bonn, Germany

### MS36 Uncertainty Quantification in Fluid Dynamics and Particle Accelerator Physics - Part II of II

### 2:00 PM-4:00 PM

Room:Ballroom E - 2nd Floor

### For Part 1 see MS28

Uncertainty quantification for simulations is a critical issue, as the models often constitute a primary source of uncertainty. We see how the specific requirements of diverse applications set the framework for justifying and assessing UQ methods. We will present and discuss the efforts to study UQ in many realistic applications from the design of particle accelerators to fusion energy to astrophysics to turbulent combustion.

Organizer: Tulin Kaman ETH Zürich and Paul Scherrer Institute, Switzerland

Organizer: James G. Glimm State University of New York, Stony Brook, USA

# 2:00-2:25 Uncertainty Quantification for Beam Dynamics Simulations

*Tulin Kaman*, ETH Zürich and Paul Scherrer Institute, Switzerland

#### 2:30-2:55 Error Analysis of Lagrangian Particle Methods

Roman Samulyak, Brookhaven National Laboratory, USA

#### 3:00-3:25 Uncertainty Quantification for Laser Driven Plasmas and Application to Astrophysical Radiative Shocks

Jean Giorla, Commissariat à l'Energie Atomique, France; Josselin Garnier, Université Paris VII, France; E. Falize, CEA/DAM/DIF, F-91297, Arpajon, France; C. Busschaert and B. Loupias, CEA, DAM, DIF-Bruyeres, France

#### 3:30-3:55 Uncertainty Quantification in Particle Accelerators: Methods and Applications

Andreas Adelmann, Paul Scherrer Institut, Switzerland

### Tuesday, April 1

## MS37

### Fast Linear Algebra for UQ in Inverse Problems and Data Assimilation - Part I of II

2:00 PM-4:00 PM

Room:Ballroom F - 2nd Floor

### For Part 2 see MS46

Large scale inverse problems and data assimilation using the Bayesian and Geo-statistical approaches are challenging because of computationally expensive "forward" models and efficient representation of high dimensional random fields. This minisymposium will focus on recent advances in fast linear algebra based computational techniques for quantifying the predictive uncertainty in large scale inverse problems and data assimilation. Methods include (but not restricted to) using efficient representation for structured matrices, such as Toeplitz and Hierarchical matrices, in combination with direct and iterative techniques to develop efficient solvers for parameter estimation and computing associated posterior uncertainty measures.

Organizer: Arvind Saibaba Tufts University, USA

Organizer: Sivaram Ambikasaran Courant Institute of Mathematical Sciences, New York University, USA

Organizer: Kenneth L. Ho Stanford University, USA

### 2:00-2:25 Hierarchical Matrix Powered Fast Kalman Filtering and Uncertainty Quantification

Sivaram Ambikasaran, Courant Institute of Mathematical Sciences, New York University, USA

# 2:30-2:55 Linear-Time Factorization of Covariance Matrices

Kenneth L. Ho and Lexing Ying, Stanford University, USA

#### 3:00-3:25 A Matern Treecode for Gaussian Process Analysis

Jie Chen, Lei Wang, and Mihai Anitescu, Argonne National Laboratory, USA

### 3:30-3:55 Uncertainty Quantification of Reservoir Performance Using Fast Reduced Order Models

Xiaochen Wang, ExxonMobil, USA

### Tuesday, April 1

# MS38

### Applications of Uncertainty Quantification in Astrodynamics - Part I of II 2:00 PM-4:00 PM

Room: Verelst Room - 2nd Floor

### For Part 2 see MS47

The operation of Earth-orbiting spacecraft has become increasingly difficult due to the proliferation of orbit debris and increased commercialization. This was made evident by several recent collisions involving operational spacecraft. Current applications of orbit trajectory uncertainty quantification seek to reduce such risks for Earthbased satellite missions, with developed techniques enabling improved tracking of debris and more accurate estimation of collision probabilities. This minisymposium will focus on uncertainty quantification-related topics specific to astrodynamics, including, but not limited to, uncertainty propagation, state estimation, and spacecraft mission design.

Organizer: Brandon A. Jones University of Colorado Boulder, USA

Organizer: Alireza Doostan University of Colorado Boulder, USA

### 2:00-2:25 Uncertainty Use and Needs in Space Situational Awareness

*Terry Alfriend*, Texas A&M University, USA; Aubrey Poore, Numerica, USA; Daniel Scheeres, University of Colorado Boulder, USA

#### 2:30-2:55 Uncertainty Quantification in Breakup and Uct Processing

*Jeff Aristoff*, Joshua Horwood, Navraj Singh, and Aubrey Poore, Numerica, USA

#### 3:00-3:25 Optimal Information Collection for Space Situational Awareness

Kumar Vishwajeet, Nagavenkat Adurthi, and *Puneet Singla*, State University of New York at Buffalo, USA

### 3:30-3:55 Coordinatization Effects on Non-Gaussian Uncertainty for Track Initialization and Refinement

*Kyle DeMars* and James McCabe, Missouri University of Science and Technology, USA

# MS39

### Low-rank and Sparse Representation Methods for Uncertainty Quantification -Part II of III

### 2:00 PM-4:00 PM

Room:Percival Room - 2nd Floor

### For Part 1 see MS31 For Part 3 see MS48

Approximations of stochastic equations may lead to extremely high dimensional problems, which may be handled by adaptive low-rank/ sparse representations. These may also be applied to statistical inverse problems of parameter identification. In addition, the solution of the forward and inverse problems can be considered as a whole adaptive process controlled by error estimators. The aim of this minisymposium is to bring together experts in adaptive methods for the discretisation and the solution of stochastic/multiparametric forward and inverse problems, and experts in low-rank/sparse tensor methods. This includes Bayesian methods, control procedures, and algorithms such as "design of experiments."

Organizer: Martin Eigel WIAS, Berlin, Germany

Organizer: Loïc Giraldi Ecole Centrale de Nantes, France

Organizer: Alexander Litvinenko King Abdullah University of Science &Technology (KAUST), Saudi Arabia

Organizer: Hermann Matthies Technische Universität Braunschweig, Germany

Organizer: Anthony Nouy Ecole Centrale de Nantes, France

### 2:00-2:25 Bayesian Compressive Sensing Framework for Sparse Representations of High-Dimensional Models

Khachik Sargsyan, Cosmin Safta, Bert J. Debusschere, and Habib N. Najm, Sandia National Laboratories, USA

### 2:30-2:55 A Least Squares Method for the Approximation of High Dimensional Functions Using Sparse Tensor Train Low-rank Format

Prashant Rai, Loïc Giraldi, and Anthony Nouy, Ecole Centrale de Nantes, France; Mathilde Chevreuil, Université de Nantes, France

### 3:00-3:25 Tensor Train Approximation of the Moment Equations for the Lognormal Darcy Problem

Fabio Nobile, EPFL, France; Francesca Bonizzoni, University of Vienna, Austria

### 3:30-3:55 Proposals Which Speed-Up Function Space Mcmc

*Kody Law*, King Abdullah University of Science & Technology (KAUST), Saudi Arabia

### Tuesday, April 1

## **MS40**

### Recent Advances of Uncertainty Quantification in Complex Environmental Applications - Part I of II

2:00 PM-4:00 PM

Room:Savannah Room - Lobby Level

### For Part 2 see MS49

Many modeling and simulation efforts in environmental applications are plagued by the many sources of uncertainties in the multi-physical modeling, nonlinear processes, high dimensionality, heterogeneous media, noisy observational data, initial and boundary conditions, and parameters, etc. These uncertainties need to be quantified systematically to gain confidence in the simulation and calibration results. This minisymposium brings together experts from several complex environmental applications to discuss the uncertainty quantification (UQ) challenges and efforts in developing and applying UQ methods to their respective applications.

Organizer: Xiao Chen Lawrence Livermore National Laboratory, USA

Organizer: Charles Tong Lawrence Livermore National Laboratory, USA

2:00-2:25 A Computational Method for Simulating Subsurface Flow and Reactive Transport in Heterogeneous Porous Media Embedded with Flexible Uncertainty Quantification

*Xiao Chen*, Brenda Ng, Yunwei Sun, and Charles Tong, Lawrence Livermore National Laboratory, USA

2:30-2:55 Bayesian Hierarchical Multiscale Model for Calibration, Validation and Uncertainty Quantification of Subsurface Flows

Matteo Icardi and Alexander Litvinenko, King Abdullah University of Science & Technology (KAUST), Saudi Arabia; Ivo Babuska and Serge Prudhomme, University of Texas at Austin, USA; Raul F. Tempone, King Abdullah University of Science & Technology (KAUST), Saudi Arabia

### 3:00-3:25 Application of Non-Intrusive Uncertainty Quantification Methods in Multiphase Flow Simulations for Coal Gasifiers

Aytekin Gel, Alpemi Consulting, LLC, USA; Mehrdad Shahnam, National Energy Technology Laboratory, USA; Arun Subramaniyan, GE Global Research, USA; Jordan Musser, National Energy Technology Laboratory, USA

#### 3:30-3:55 A Flexible and Modular Framework for Uncertainty Quantification in Non-Linearly Coupled Multi-Physics Applications

Akshay Mittal, Stanford University, USA; Xiao Chen, Lawrence Livermore National Laboratory, USA; Gianluca Iaccarino, Stanford University, USA; Charles Tong, Lawrence Livermore National Laboratory, USA

### Tuesday, April 1

### MS41 Sensitivity Analysis and Calibration of Climate Models

### 2:00 PM-4:00 PM

Room: Plimsoll - Lobby Level

Uncertainty quantification of climate models is vital as we shift from explaining climate to predicting it. In order to explain complex climate processes parameterisations are added to existing computer code aiming for better comparison to observations. To predict with these complex computer codes the whole suite of parameterisations must work together to simulate real world processes and their interactions. Sensitivity analysis and calibration compare ensembles to observations identifying when and how the computer code represents reality. This is important for model development and producing trustworthy predictions. We will show the latest applications of sensitivity analysis and calibration to climate models.

### Organizer: Lindsay Lee University of Leeds, United Kingdom

2:00-2:25 Sensitivity Analysis and Calibration a Global Aerosol Model *Lindsay Lee*, Ken Carslaw, Kirsty Pringle,

Carly Reddington, and Graham Mann, University of Leeds, United Kingdom

#### 2:30-2:55 History Matching for the Identification and Removal of Structural Errors in Climate Models

Danny Williamson, Durham University, United Kingdom

### 3:00-3:25 The Potential of An Observational Data Set for Calibration of a Computationally Expensive Computer Model Doug McNeall, Met Office, United Kingdom

#### 3:30-3:55 Calibration of Waccm's Gravity Waves Parametrizations Using Spherical Outputs

Kai-Lan Chang and Serge Guillas, University College London, United Kingdom; Hanli Liu, National Center for Atmospheric Research, USA

### Tuesday, April 1

### CP9 Bayesian Approaches 2:00 PM-3:20 PM

Room: Vernon Room - 2nd Floor

Chair: Nicholas Zabaras, Cornell University, USA

#### 2:00-2:15 Calibration and Confidence Assessment of Transient, Coupled Models Using Dynamic Bayesian Networks

*Erin C. Decarlo* and Sankaran Mahadevan, Vanderbilt University, USA; Benjamin P. Smarslok, Air Force Research Laboratory, USA

#### 2:20-2:35 Variational Bayesian Approximations for Nonlinear Inverse Problems

Phaedon S. Koutsourelakis and *Isabell Franck*, Technische Universität München, Germany

#### 2:40-2:55 Bayesian Experimental Design for Stochastic Kinetic Models

*Colin Gillespie*, Newcastle University, United Kingdom

#### 3:00-3:15 Solution of Inverse Problems with Limited Forward Solver Evaluations: A Bayesian Perspective Nicholas Zabaras and Ilias Bilionis, Cornell

Vicholas Zabaras and Ilias Bilionis, Corn University, USA

## CP10 Algorithms II

2:00 PM-4:00 PM

Room:Sloane Room - 2nd Floor

Chair: Ilias Bilionis, Purdue University, USA

#### 2:00-2:15 Design of Polynomial Chaos Basis for Sparse Approximation of Stochastic Functions

Ji Peng, Dave Biagioni, and Alireza Doostan, University of Colorado Boulder, USA; Dongbin Xiu, University of Utah, USA

### 2:20-2:35 Pc-Kriging: the Best of Polynomial Chaos Expansions and Gaussian Process Modelling

Bruno Sudret and Schoebi Roland, ETH Zürich, Switzerland

#### 2:40-2:55 Guarantees of Near-Optimal Experimental Input Design for System Identification

AlbertoGiovanni Busetto and John Lygeros, ETH Zürich, Switzerland

#### 3:00-3:15 Enhanced Predictive Capability of Surrogate Models Through Model Selection

Nicholas Zabaras and Jesper Kristensen, Cornell University, USA

# 3:20-3:35 Multi-Fidelity Wavelet Regression.

*Federico Zertuche*, Université de Grenoble I, France; Celine Helbert, Institut Camille Jordan, France; Anestis Antoniadis, Universite Joseph Fourier, France

### 3:40-3:55 Generation of Uncertainty-Based Analytics for Selected Problems in Aerospace Systems Technology Transition

R

*Rick Graves*, U.S. Air Force Research Laboratory, USA

### **Coffee Break**



Room:Regency Foyer and Promenade - 2nd Floor

### Tuesday, April 1

### **MS42**

The Reliability of Computational Research Findings: Reproductible Research, Uncertainty Quantification, and Verification & Validation 4:30 PM-6:30 PM

Room:Ballroom A - 2nd Floor

Reproducibility has become a topic of recent interest, as researchers define and implement practices to enable others to replicate computational findings and compare performance and results. A 2012 Workshop Report listed best practice criteria for a computational publication to be considered reproducible research. One of these was "verification and validation (V&V) tests performed by the author(s)." Uncertainty Quantification can also be considered an important aspect of reproducibility when it's impossible to duplicate results exactly. The overlap between creating reproducible research and UQ isn't well-understood. This panel will explore the contours of these areas and shape an informed research agenda. This session is designed to complement MT4.

Organizer: Victoria Stodden Columbia University, USA

4:30-4:55 An Overview of Reproducible Research, Uq, and V&V Victoria Stodden, Columbia University, USA

#### 5:00-5:25 Uq and Reliability of Computational Results Habib N. Najm, Sandia National

Laboratories, USA

#### 5:30-5:55 Relating Reproducible Research and Uq

*Philip Stark*, University of California, Berkeley, USA

6:00-6:25 Reproducible Research and Uq in the SuperComputing Context Lorena A. Barba, Boston University, USA

### Tuesday, April 1

## **MS43**

### Numerical Approximation of High-dimensional Stochastic Equations -Part IV of IV

4:30 PM-6:00 PM

Room:Ballroom B - 2nd Floor

### For Part 3 see MS34

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 are affected by large amounts of uncertainty. For higher accuracy in computational simulations, approximations must increase the number of random variables (dimensions), and expend more effort resolving smooth or even discontinuous behavior within each individual dimension. The resulting explosion in computational effort is a symptom of the efforts effort is a symptom of curse of dimensionality. This minisymposium aims at exploring efforts related to efficient stochastic Galerkin, collocation and Monte Carlo finite element methods, error analysis, anisotropy and adaptive methods, multi-level and multiresolution analysis, random sampling and sparse grids.

Organizer: Clayton G. Webster Oak Ridge National Laboratory, USA

Organizer: Michael Griebel Universitaet Bonn, Germany

#### 4:30-4:55 Multilevel Quadrature for Elliptic Stochastic Partial Differential Equations

Helmut Harbrecht, Universität Basel, Switzerland

#### 5:00-5:25 Multilevel Estimation of Rare Events

*Elisabeth Ullmann*, University of Bath, United Kingdom; Iason Papaioannou, TU Munich, Germany

#### 5:30-5:55 Convergence Analysis for Multilevel Sample Variance Estimators and Application for Random Obstacle Problems

Alexey Chernov and Claudio Bierig, University of Reading, United Kingdom

## **MS44**

### Adaptive Methods in Uncertainty Quantification -Part II of II

4:30 PM-6:30 PM

Room:Ballroom D - 2nd Floor

### For Part 1 see MS35

The computational demand of single simulation runs poses limits to the quantification of uncertainties, especially with non-intrusive methods that aim to approximate the response surface for the problem at hand. Numerical approximations suffer from the curse of dimensionality, and most problems demand high resolution only in certain parameter ranges. To reduce the computational demand, an adaptive representation and exploration of such response surfaces is required. Typical applications encounter non-smooth parameter dependencies or even shock phenomena, such as when measuring leakage at a fault in a cap rock for subsurface flows. This minisymposium addresses the current state of the art of adaptive approaches for non-intrusive methods in uncertainty quantification.

Organizer: Dirk Pflüger Universität Stuttgart, Germany

Organizer: John D. Jakeman Sandia National Laboratories, USA

Organizer: Tobias Neckel *TU München, Germany* 

4:30-4:55 Sensitivity Analysis in Multivariate Peridynamics Simulations with the Adaptive Sparse Grid Collocation Method

Fabian Franzelin, Universität Stuttgart, Germany; Patrick Diehl, Universität Bonn, Germany; Dirk Pflüger, Universität Stuttgart, Germany

### 5:00-5:25 Accelerated Hierarchical Stochastic Collocation Methods for PDEs with Random Inputs

*Diego Galindo*, Clayton G. Webster, and Guannan Zhang, Oak Ridge National Laboratory, USA

### 5:30-5:55 Adaptive Basis Selection Methods for Enhancing Compressive Sensing

Michael S. Eldred, Sandia National Laboratories, USA

### 6:00-6:25 Integrated Variance as an Experimental Design Objective for Gaussian Process Regression

Alex A. Gorodetsky and Youssef M. Marzouk, Massachusetts Institute of Technology, USA

### Tuesday, April 1

## MS45 Inverse Problems in Cardiovascular Mathematics

4:30 PM-6:30 PM

### Room:Ballroom E - 2nd Floor

We present inverse problems arising in the numerical simulation of the cardiovascular system dealing with data assimilation, parameter estimation, shape registration and reconstruction. We focus on robust optimization techniques to take into account uncertainties in some parameters (flow rates, flow residuals, arterial and blood physical properties, etc) and we take into account also reduced order modelling and computational reduction techniques to improve computational performances in bio-medicine. This session is designed to complement MT3.

Organizer: Gianluigi Rozza SISSA, International School for Advanced Studies, Trieste, Italy

### 4:30-4:55 Bayesian Inversion for Data Assimilation in Hemodynamics

Marta D'Elia, Florida State University, USA; Alessandro Veneziani, Emory University, USA

#### 5:00-5:25 Computational Models for Coupling 3d-1d Flow and Mass Transport Problems Applied to Shape Sensitivity Analysis and Numerical Homogenization of Vascular Networks

Laura Cattaneo, Politecnico di Milano, Italy; Paolo Zunino, University of Pittsburgh, USA

#### 5:30-5:55 Blood Velocity Profile Estimation Via Spatial Regression with Pde Penalization

Laura Azzimonti, Politecnico di Milano, Italy; *Fabio Nobile*, EPFL, France; Laura M. Sangalli and Piercesare Secchi, Politecnico di Milano, Italy

#### 6:00-6:25 Fractional-Order Viscoelasticity in One Dimensional Blood Flow Models

Paris Perdikaris and George E. Karniadakis, Brown University, USA

# **MS46**

### Fast Linear Algebra for UQ in Inverse Problems and Data Assimilation - Part II of II

4:30 PM-6:30 PM

Room:Ballroom F - 2nd Floor

### For Part 1 see MS37

Large scale inverse problems and data assimilation using the Bayesian and Geo-statistical approaches are challenging because of computationally expensive "forward" models and efficient representation of high dimensional random fields. This minisymposium will focus on recent advances in fast linear algebra based computational techniques for quantifying the predictive uncertainty in large scale inverse problems and data assimilation. Methods include (but not restricted to) using efficient representation for structured matrices, such as Toeplitz and Hierarchical matrices, in combination with direct and iterative techniques to develop efficient solvers for parameter estimation and computing associated posterior uncertainty measures.

Organizer: Arvind Saibaba *Tufts University, USA* 

Organizer: Sivaram Ambikasaran Courant Institute of Mathematical Sciences, New York University, USA

Organizer: Kenneth L. Ho Stanford University, USA

#### 4:30-4:55 Fast Kalman Filter Using Hierarchical Matrices and Low-Rank Perturbative Approach

Arvind Saibaba, Tufts University, USA; Peter K Kitanidis, Stanford University, USA

#### 5:00-5:25 Improving Computational Efficiency in Large Linear Inverse Problems: An Example from Carbon Dioxide Flux Estimation

Vineet Yadav and Anna Michalak, Carnegie Institution for Science, USA

#### 5:30-5:55 Geostatistical Reduced-Order Models in Inverse Problems

*Xiaoyi Liu*, Quanlin Zhou, and Jens T. Birkholzer, Lawrence Berkeley National Laboratory, USA

#### 6:00-6:25 Compressed State Kalman Filter for Large Systems

Peter K. Kitanidis, Stanford University, USA

## Tuesday, April 1

## **MS47**

## Applications of Uncertainty Quantification in Astrodynamics - Part II of II

4:30 PM-6:30 PM

Room: Verelst Room - 2nd Floor

### For Part 1 see MS38

The operation of Earth-orbiting spacecraft has become increasingly difficult due to the proliferation of orbit debris and increased commercialization. This was made evident by several recent collisions involving operational spacecraft. Current applications of orbit trajectory uncertainty quantification seek to reduce such risks for Earthbased satellite missions, with developed techniques enabling improved tracking of debris and more accurate estimation of collision probabilities. This minisymposium will focus on uncertainty quantification-related topics specific to astrodynamics, including, but not limited to, uncertainty propagation, state estimation, and spacecraft mission design.

Organizer: Brandon A. Jones University of Colorado Boulder, USA

Organizer: Alireza Doostan University of Colorado Boulder, USA

#### 4:30-4:55 High-Dimension Orbit Uncertainty Propagation Using Separated Representations

*Marc Balducci*, Brandon A. Jones, and Alireza Doostan, University of Colorado Boulder, USA

### 5:00-5:25 Uncertainty Propagation Using Gaussian Mixture Models

Vivek Vittaldev and Ryan Russell, University of Texas at Austin, USA

#### 5:30-5:55 Sparse Grid Based Forward and Inverse Orbit Uncertainty Quantification

Yang Cheng, Mississippi State University, USA; Yang Tian, Harbin Institute of Technology, China

#### 6:00-6:25 Collision Risk Estimation for the Magnetospheric Multiscale Mission Using Polynomial Chaos Expansions

Brandon A. Jones, University of Colorado Boulder, USA

### Tuesday, April 1

## **MS48**

### Low-rank and Sparse Representation Methods for Uncertainty Quantification -Part III of III

4:30 PM-6:30 PM

Room:Percival Room - 2nd Floor

### For Part 2 see MS39

Approximations of stochastic equations may lead to extremely high dimensional problems, which may be handled by adaptive low-rank/ sparse representations. These may also be applied to statistical inverse problems of parameter identification. In addition, the solution of the forward and inverse problems can be considered as a whole adaptive process controlled by error estimators. The aim of this minisymposium is to bring together experts in adaptive methods for the discretisation and the solution of stochastic/multiparametric forward and inverse problems, and experts in low-rank/sparse tensor methods. This includes Bayesian methods, control procedures, and algorithms such as "design of experiments."

Organizer: Martin Eigel WIAS, Berlin, Germany

Organizer: Loïc Giraldi Ecole Centrale de Nantes, France

Organizer: Alexander Litvinenko King Abdullah University of Science &Technology (KAUST), Saudi Arabia

Organizer: Hermann Matthies Technische Universität Braunschweig, Germany

Organizer: Anthony Nouy Ecole Centrale de Nantes, France

#### 4:30-4:55 A Randomized Tensor Algorithm for the Construction of Green's Functions for Elliptic sPDE's

David Biagioni and Alireza Doostan, University of Colorado Boulder, USA; Gregory Beylkin, University of Colorado, USA

### 5:00-5:25 Rank Reduction of Parameterized Time-dependent PDEs

Alessio Spantini, Massachusetts Institute of Technology, USA; Lionel Mathelin, CNRS, France; Youssef M. Marzouk, Massachusetts Institute of Technology, USA

### 5:30-5:55 On the Convergence of Alternating Optimisation in Tensor Format Representations

Mike Espig, Max Planck Institute, Germany

#### 6:00-6:25 Dynamical Low Rank Approximation in Hierarchical Tensor Formats

*Reinhold Schneider*, Technische Universität Berlin, Germany

### Tuesday, April 1

## **MS49**

### Recent Advances of Uncertainty Quantification in Complex Environmental Applications - Part II of II

4:30 PM-6:30 PM

Room:Savannah Room - Lobby Level

### For Part 1 see MS40

Many modeling and simulation efforts in environmental applications are plagued by the many sources of uncertainties in the multi-physical modeling, nonlinear processes, high dimensionality, heterogeneous media, noisy observational data, initial and boundary conditions, and parameters, etc. These uncertainties need to be quantified systematically to gain confidence in the simulation and calibration results. This minisymposium brings together experts from several complex environmental applications to discuss the uncertainty quantification (UQ) challenges and efforts in developing and applying UQ methods to their respective applications.

Organizer: Xiao Chen Lawrence Livermore National Laboratory, USA

Organizer: Charles Tong Lawrence Livermore National Laboratory, USA

#### 4:30-4:55 Exploring Parametric Uncertainty of Weather Research and Forecasting Model

Zhenhua Di, *Qingyun Duan*, Jiping Quan, Wei Gong, and Chen Wang, Beijing Normal University, China

#### 5:00-5:25 Uncertainty Quantification and Risk Mitigation of CO<sup>2</sup> Leakage in Groundwater Aquifers

*Yunwei Sun*, Lawrence Livermore National Laboratory, USA

#### 5:30-5:55 A UQ Framework for Carbon Capture Process Models

*Charles Tong,* Brenda Ng, and Jeremy Out, Lawrence Livermore National Laboratory, USA

### 6:00-6:25 Updating Reservoir Models by Transient Well Test Data

Hamidreza Hamdi, University of Calgary, Canada

### Tuesday, April 1

## MS50 Sequential and Adaptive Monte Carlo Methods

### 4:30 PM-6:30 PM

Room:Plimsoll - Lobby Level

Sequential and adaptive particle methods are well suited tools for exploring probability distributions, in particular when they evolve over time and data acquisition is done dynamically. The talks in this minisymposium will present an overview of recent progress aimed at increasing the effectiveness and efficiency of sequential and adaptive Monte Carlo methods.

Organizer: Daniela Calvetti Case Western Reserve University, USA

Organizer: Erkki Somersalo Case Western Reserve University, USA

#### 4:30-4:55 Estimating Innovation Variance in Sequential MC from Numerical Integration Error

Daniela Calvetti, Andrea N. Arnold, and Erkki Somersalo, Case Western Reserve University, USA

#### 5:00-5:25 Mathematical Theory for Filtering with Model Errors

*Tyrus Berry*, George Mason University, USA; John Harlim, Pennsylvania State University, USA

#### 5:30-5:55 Adaptive Metropolis Algorithm Using Variational Bayesian Adaptive Kalman Filter

Isambi S. Mbalawata, Lappeenranta University of Technology, Finland

#### 6:00-6:25 Sequential Statistical Inference in State-space Models Using SMC<sup>2</sup>

*Omiros Papaspiliopoulos*, Universitat Pompeu Fabra, Spain

## CP11 **Reduced-order Modelina**

4:30 PM-6:10 PM

Room: Vernon Room - 2nd Floor

Chair: Irina Kalashnikova, Sandia National Laboratories, USA

### 4:30-4:45 Bayesian Reduced-Basis Models

Phaedon S. Koutsourelakis, Technische Universität München, Germany

### 4:50-5:05 Goal-Oriented Error Estimation for Reduced Basis Method

Alexandre Janon, Université Paris-Sud, France; Clementine Prieur and Maelle Nodet, Universite Joseph Fourier and INRIA, France

### 5:10-5:25 Stabilized Projection-Based **Reduced Order Models for Uncertainty** Quantification

Irina Kalashnikova, Bart Vanbloemenwaanders, Srinivasan Arunajatesan, and Matthew Barone, Sandia National Laboratories, USA

### 5:30-5:45 Optimal Reduced Basis for **Vector-Valued Stochastic Processes** Defined by a Set of Realizations

Guillaume Perrin, Christian Soize, and Denis Duhamel, Université Paris-Est, France; Christine Funfschilling, SNCF, France

### 5:50-6:05 A Model Reduction Algorithm for a Class of Stochastic Configurations

Mahadevan Ganesh, Colorado School of Mines, USA; Stuart Hawkins, Macquarie University, Sydney, Australia

### Tuesday, April 1

## **CP12 Models and Algorithms**

4:30 PM-6:10 PM

Room:Sloane Room - 2nd Floor

Chair: Chen Liang, Vanderbilt University, USA

### 4:30-4:45 Fuzzy Risk Analysis Based on Ranking Fuzzy Numbers

Tayebeh Hajjari, Islamic Azad University, Iran

### 4:50-5:05 Building Metamodels for Stochastic Simulation Codes

Bertrand Iooss and Vincent Moutoussamy, EDF. France: Simon Nanty. Commissariat à l'Energie Atomique, France; Pauwel Benoit and Delbos Frédéric, IFPEN. France: Marrel Amandine, CEA, France

### 5:10-5:25 Stochastic Multi-Disciplinary Analysis under Data Uncertainty and **Model Error**

Chen Liang, Vanderbilt University, USA; Shankar Sankararaman, NASA Ames Research Center, USA; Sankaran Mahadevan, Vanderbilt University, USA

### 5:30-5:45 An Origin of Macroscopic Uncertainty/randomness

Shijun Liao, Shanghai Jiao Tong University, China

#### 5:50-6:05 Application of the Polynomial Chaos Technique for Global Sensitivity Analysis in a Finite Element Model for Deep Brain Stimulation

Christian Schmidt and Ursula Van Rienen, University of Rostock, Germany

### **Dinner Break**

6:30 PM-8:00 PM

Attendees on their own

### SIAG/UQ Business Meeting

8:00 PM-8:45 PM

Room:Ballroom A - 2nd Floor

Complimentary beer and wine will be served

# Wednesday, April 2

### Registration

7:30 AM-5:00 PM Room: Registration Booth - 2nd Floor

### Remarks

8:10 AM-8:15 AM Room:Ballroom A/B/C - 2nd Floor

# IP5

### **Gaussian Process Emulation** of Computer Models with **Massive Output**

8:15 AM-9:00 AM

Room:Ballroom A/B/C - 2nd Floor

Chair: Kerstin Lehnert, Lamont Doherty Earth Observatory, Columbia University, USA

Often computer models yield massive output, such as temperature over a large grid of space and time. Emulation (i.e., developing a fast approximation) of the computer model can then be particularly challenging. Approaches that have been considered include utilization of multivariate emulators, modeling of the output (e.g., through some basis representation, including PCA), and construction of parallel emulators at each grid point. These approaches will be reviewed, with the startling computational simplicity with which the last approach can be implemented being highlighted. Illustrations with computer models of pyroclastic flow and wind fields will be given.

James Berger (speaker) Mengyang Gu Duke University, USA

### **Coffee Break**



Room:Regency Foyer and Promenade - 2nd Floor

9:00 AM-9:30 AM

(E)

## MT5

### Estimation of Prediction Uncertainties in Oil Reservoir Simulation using Bayesian and Proxy Modeling Techniques

9:30 AM-11:30 AM

Room:Ballroom A - 2nd Floor Chair: Ralf Schulze-Riegert, Schlumberger, Norway

Subsurface uncertainties have a large impact on oil & gas production forecasts. Underestimation of prediction uncertainties therefore presents a high risk to investment decisions for facility designs and exploration targets. The complexity and computational cost of reservoir simulation models often defines narrow limits for the number of simulation runs used in related uncertainty quantification studies. In this minitutorial we will look into workflow designs and methods that have proven to deliver results in industrial reservoir simulation workflows. Combinations of automatic proxy modeling, MCMC and Bayesian approaches for estimating prediction uncertainties are presented.

Ralf Schulze-Riegert, Schlumberger, Norway

Wednesday, April 2

## **MS51**

### Numerical Methods for Uncertainty Quantification of Coupled Problems -Part I of V

9:30 AM-11:30 AM

Room:Ballroom B - 2nd Floor

### For Part 2 see MS70

Accurate prediction of many engineering systems often requires simulations of tightly coupled and interacting phenomena with multiple physics or domains and at multiple scales. When uncertainties are present, the UQ of such coupled systems is challenged by two difficulties. First, the presence of independent uncertainty sources within different physics/ scale models results in a combined high- dimensional stochastic space which may not be amenable to fast computation using standard approaches. Second, single physics/scale solvers are separate modules that may not have access to detailed information from one another. This minisymposium invites contributions that discuss the above challenges and provide novel solution techniques.

Organizer: Alireza Doostan University of Colorado Boulder, USA

Organizer: Dongbin Xiu University of Utah, USA

### 9:30-9:55 Localized Polynomial Chaos Expansion for Differential Equations with Random Inputs

Yi Chen and Claude J. Gittelson, Purdue University, USA; *Dongbin Xiu*, University of Utah, USA

### 10:00-10:25 Noise Propagation and Uncertainty Quantification in Hybrid Multiphysics Models

Daniel M. Tartakovsky and Soren Taverniers, University of California, San Diego, USA; Francis Alexander, Los Alamos National Laboratory, USA

### 10:30-10:55 A Stochastic Collocation Approach for Multi-Fidelity Model Classes

Akil Narayan, University of Massachusetts, Dartmouth, USA; Xueyu Zhu and Dongbin Xiu, University of Utah, USA; Claude J. Gittelson, Purdue University, USA

#### 11:00-11:25 Multilevel and Weighted Reduced Basis Method for Optimal Control Problems Constrained by Stochastic PDEs

Peng Chen and Alfio Quarteroni, École Polytechnique Fédérale de Lausanne, Switzerland; Gianluigi Rozza, SISSA, International School for Advanced Studies, Trieste, Italy

## **MS52**

### Uncertainty Quantification in Well Constructed Mathematical Models in Epidemiology

### 9:30 AM-11:30 AM

### Room:Ballroom D - 2nd Floor

Despite of constructing mathematical models for understanding various purposes in epidemiology, there is an amount of uncertainty that is outside the control of epidemiologists and mathematicians. This uncertainty could dilute the desired accuracy with which a good mathematical model is expected to function either in predicting an epidemic or impact of interventions in epidemic control. We first motivate for theoretical ideas in quantifying uncertainty and then bring checklist of handling various uncertainties. There could be several uncertainties due to flaws in model building or poor understanding of biological processes, but we restrict our focus to uncertainties in carefully built mathematical models in epidemiology.

Organizer: Arni S.R. Sri.R. Srinivasa Rao

Georgia Regents University, USA

#### 9:30-9:55 Uncertainties in Carefully Constructed Models in Epidemiology

Roy M. Anderson, Imperial College London, United Kingdom

# 10:00-10:25 Not available at time of publication

Hiroshi Nishiura, University of Tokyo, Japan

10:30-10:55 Not available at time of publication

Greg Rempala, Ohio State University, USA

#### 11:00-11:25 Set Theoretic Approaches in Uncertainty Measures

Arni S.R. Sri.R. Srinivasa Rao, Georgia Regents University, USA Wednesday, April 2

## MS53

### Data Assimilation in Atmospheric and Oceanographic Processes 9:30 AM-11:30 AM

Room:Ballroom E - 2nd Floor

Data assimilation describes a broad range of techniques to combine physical models and observations of a system. Often, the model underlying a geophysical process (atmosphere, oceans, etc.) is a dynamical system. Such systems may be highly nonlinear, chaotic, and/or very high-dimensional. The general framework for data assimilation involves an uncertain state variable that changes in time, combined with noisy observations of that state. This session will focus on ensemble and hybrid data assimilation methods in several contexts, including Lagrangian data assimilation and parameter estimation.

Organizer: Adam B. Mallen Marquette University, USA

Organizer: Laura Slivinski Brown University, USA

9:30-9:55 The Effect of Targeted Observations with the Kalman Filter: Linear Analysis and Model Problems Thomas Bellsky, Arizona State University, USA

### 10:00-10:25 Thinking Locally: Estimating spatially-varying parameters using LETKF

Jesse Berwald, University of Minnesota, USA; Thomas Bellsky, Arizona State University, USA; Lewis Mitchell, University of Vermont, USA

#### 10:30-10:55 A Hybrid Particle-Ensemble Kalman Filter Scheme for Lagrangian Data Assimilation Laura Slivinski, Brown University, USA

11:00-11:25 Assimilation of Ocean Glider Data in a 3-D Flow Model Adam B. Mallen, Marquette University, USA

### Wednesday, April 2

## **MS54**

### Active Subspace Methods for High-dimensional Approximation and Inverse Problems - Part I of II

9:30 AM-11:30 AM

Room:Ballroom F - 2nd Floor

### For Part 2 see MS63

Most methods for uncertainty quantification struggle with highdimensional parameter spaces due to the curse of dimensionality. Sensitivity analysis can reduce the dimension by identifying the important parameters, which enables UQ studies. However, most sensitivity analysis methods are restricted to the original parameters. Active subspace methods identify and exploit a set of directions---i.e., linear combinations of the original parameters---that are most important for approximation. This minisymposium explores the use of active subspace methods for (i) approximating functions of many parameters and (ii) solving inverse UQ problems with highdimensional inputs.

Organizer: Paul Constantine Colorado School of Mines, USA

# 9:30-9:55 Active Subspace Methods in Theory and Practice

*Eric Dow*, Massachusetts Institute of Technology, USA

# 10:00-10:25 Dimension Reduction in Nonlinear Statistical Inverse Problems

James R. Martin, University of Texas at Austin, USA; Tiangang Cui, Massachusetts Institute of Technology, USA; Tarek Moselhy, Massachusetts Institute of Technology, USA; Omar Ghattas, University of Texas at Austin, USA; Youssef M. Marzouk, Massachusetts Institute of Technology, USA

#### 10:30-10:55 An Active Space Method for Exploring High Dimensional Bayesian Posterior Density

Matteo Giacomini and Tan Bui-Thanh, University of Texas at Austin, USA

# 11:00-11:25 Subspace Adaptation in Polynomial Chaos Spaces

Roger Ghanem, University of Southern California, USA; *Ramakrishna Tipireddy*, Pacific Northwest National Laboratory, USA

### MS55 Advances in Optimal Experimental Design -Part I of IV

9:30 AM-11:00 AM

Room: Verelst Room - 2nd Floor

### For Part 2 see MS64

The challenge of optimal information gathering---reflecting some end goal of inference, prediction, or control---pervades fields ranging from geophysics to systems biology to autonomy. Extending classical Bayesian experimental design methodologies to tackle problems of greater scale and dynamic complexity requires new algorithms and even new formulations. This minisymposium aims to cross-fertilize a wide variety of methodologies, where key challenges include: (1) design for ill- posed and large-scale inverse problems, nonlinear models, design in the presence of model error, and the estimation of information gain; and (2) optimal closed-loop (sequential) experimental design, harnessing rigorous approaches developed in multiple communities (e.g., controls, statistics, operations research).

Organizer: Xun Huan Massachusetts Institute of Technology, USA

Organizer: Youssef M. Marzouk Massachusetts Institute of Technology, USA

Organizer: Luis Tenorio Colorado School of Mines, USA

Organizer: Gabriel A. Terejanu University of Texas at Austin, USA

### 9:30-9:55 Bayesian Experimental Design in the Presence of Model Error

*Xiao Lin* and Gabriel Terejanu, University of South Carolina, USA

#### 10:00-10:25 Optimal Experimental Design and Model Misspecification Mitigation

*Lior Horesh*, IBM T.J. Watson Research Center, USA

#### 10:30-10:55 Real Time Optimal Experimental Design for Joint Flow and Geophysical Imaging of Dynamic Targets

Jennifer Fohring and Eldad Haber, University of British Columbia, Canada

### Wednesday, April 2

## MS56 Efficient Simulation of Rare Events - Part I of IV

9:30 AM-11:30 AM

Room:Percival Room - 2nd Floor

### For Part 2 see MS65

Applications in materials science, theoretical chemistry, and atmosphere science call for efficient algorithms for simulation of rare events. The study of such events is crucial since they lead to important understanding of the system, for example, the failure of materials, the phase transition, chemical reaction, etc. Recent advances use ideas from importance sampling, large deviation theory, extreme value analysis, and uncertainty quantification. This minisymposium aims at bringing together experts and young researchers to discuss recent development and future directions. Topics include large deviation, importance sampling, discontinuity/edge detection, stochastic optimization/control, transition pathway, with applications in engineering, physics, biology and materials science.

Organizer: Xiang Zhou City University of Hong Kong, Hong Kong

Organizer: Jianfeng Lu Duke University, USA

Organizer: Jingchen Liu Columbia University, USA

Organizer: Richard Archibald Oak Ridge National Laboratory, USA

Organizer: Guannan Zhang Oak Ridge National Laboratory, USA

#### 9:30-9:55 The Importance Sampling Technique for Understanding Rare Events in Erdos-Renyi Random Graphs

*Chia Ying Lee*, University of British Columbia, Canada and University of North Carolina, USA; Shankar Bhamidi and Jan Hannig, University of North Carolina, USA; James Nolen, Duke University, USA

#### 10:00-10:25 Selection of Polynomial Chaos Bases Via Bayesian Mixed Shrinkage Prior Model with Applications to Sparse Approximation of Pdes with Stochastic Inputs

*Georgios Karagiannis*, Bledar Konomi, and Guang Lin, Pacific Northwest National Laboratory, USA

10:30-10:55 An Explicit Cross-Entropy Method for Mixture

Hui Wang, Brown University, USA

11:00-11:25 A Low-Order Stochastic Model for Flow Control Problem Ju Ming, Florida State University, USA

### MS57 Uncertainty Quantification Driven by Large-Scale Applications

### 9:30 AM-11:30 AM

### Room:Sloane Room - 2nd Floor

Since the importance of uncertainty quantification has been understood by the mathematics and engineering communities in this decade, key principles, methodologies and tools have been developed and are evolving for predictive science and engineering. At the same time, the development of high-performance scientific computing has been significantly improving the capabilities for solving UQ problems in applications, e.g. climate modeling and turbulence computation. This minisymposium aims at exploring recent efforts related to theories and computations of uncertainty quantification driven by large-scale applications. Specific topics includes scalable algorithms for UQ, model calibration, parameter estimation, data-driven reduced order method.

Organizer: Guannan Zhang Oak Ridge National Laboratory, USA

Organizer: Clayton G. Webster Oak Ridge National Laboratory, USA

#### 9:30-9:55 Stochastic Parameterization of Sub-Grid Latent Heat Flux for Climate Models

*Roisin T. Langan* and Richard Archibald, Oak Ridge National Laboratory, USA; Matthew Plumlee, Georgia Institute of Technology, USA; Salil Mahajan, Rui Mei, Jaifu Mao, and Daniel Ricciuto, Oak Ridge National Laboratory, USA; Joshua Fu and Cheng-En Yang, University of Tennessee, Knoxville, USA

#### 10:00-10:25 Multilevel Acceleration of Stochastic Collocation Methods for SPDEs

Peter Jantsch, University of Tennessee, USA; Aretha L. Teckentrup and Max Gunzburger, Florida State University, USA; Clayton G. Webster, Oak Ridge National Laboratory, USA

### 10:30-10:55 Optimal Point Sets for Interpolation of Total Degree Polynomials in Moderate Dimensions

Aretha L. Teckentrup and Max Gunzburger, Florida State University, USA

11:00-11:25 Bayesian Inference for An Eddy Viscosity-Type Les Models in Simulation of Turbulent Flow Around a Cylinder

Hoang A. Tran, Clayton G. Webster, and Guannan Zhang, Oak Ridge National Laboratory, USA Wednesday, April 2

# MS58

### Data-centered and Gridbased Non-parametric Probability Density Estimation

9:30 AM-11:30 AM

Room:Savannah Room - Lobby Level

Probability density estimation is a ubiquitous task in UQ. For example, instead of storing a large number of data samples, it is often cheaper to estimate the density first and then sample from it later when data is needed. Usually, the non-parametric kernel density estimation (KDE) method is employed which uses only the given data and does not require any additional knowledge. However, in its pure form, KDE is very sensitive to parameters (bandwidth), and it can become slow for large data sets. We present several improvements of and alternatives to standard KDE which have a wide applicability in UQ-related problems.

Organizer: Benjamin Peherstorfer Massachusetts Institute of Technology, USA

Organizer: Markus Hegland Australian National Unversity, Canberra, Australia

Organizer: Dirk Pflüger Universität Stuttgart, Germany

9:30-9:55 Density Estimation with Adaptive Sparse Grids

Benjamin Peherstorfer, Massachusetts Institute of Technology, USA

10:00-10:25 Speeding Up the Evaluation of Kernel Density Estimators Zdravko Botev, University of New South Wales, Australia

10:30-10:55 Density Estimation Trees Parikshit Ram, Skytree, Inc., USA

#### 11:00-11:25 A Finite Element Method for Density Estimation with Gaussian Process Priors

Markus Hegland, Australian National Unversity, Canberra, Australia

## **MS59**

### UQ for Inverse Problems: Data Assimilation, Parameter Estimation, and Sampling -Part I of III

9:30 AM-11:30 AM

Room: Plimsoll - Lobby Level

### For Part 2 see MS68

In inverse problems, parameters in a physical model are estimated from indirect measurements. Due to modeling errors and random noise in the measurement process, any estimator of the unknown parameters is a random quantity, and hence quantifying uncertainty in the estimator is an important task. In this minisymposium, the talks focus on techniques for uncertainty quantification in inverse problems. The topics considered include classical applications in inverse problems, such as x-ray radiography and electrical impedance tomography; parameter estimation for ODE models; data assimilation for weather prediction; and Monte Carlo sampling methods.

Organizer: Johnathan M. Bardsley University of Montana, USA

### 9:30-9:55 Distance Metrics for Chaotic Systems

Heikki Haario, Lappeenranta University of Technology, Finland; Janne Hakkarainen, Finnish Meteorological Institute, Helsinki, Finland; Leonid Kalachev, University of Montana, USA

### 10:00-10:25 Experiences with Parameter Estimation in Chaotic Models

Antti Solonen, Lappeenranta University of Technology, Finland

#### 10:30-10:55 Bayesian Model Calibration in the Presence of Model Discrepancy

Ralph C. Smith and Jerry McMahan, North Carolina State University, USA

### 11:00-11:25 A Bayesian Approach to Hyperspectral Remote Sensing of Canopy LAI

Petri Varvia and Aku Seppanen, University of Eastern Finland, Finland; Miina Rautiainen, University of Helsinki, Finland Wednesday, April 2

## **CP13** Geophysical Flows

9:30 AM-11:30 AM

Room: Vernon Room - 2nd Floor

Chair: Pierre Sochala, BRGM, France

### 9:30-9:45 Emulation of Complex Simulator Models with Application to Hydrology

David Machac, ETH Zürich, Switzerland; Peter Reichert, Swiss Federal Institute of Aquatic Science and Technology, Switzerland; Carlo Albert, Eawag, Switzerland

#### 9:50-10:05 Polynomial Chaos Expansion for Subsurface Flows with Uncertain Soil Parameters

*Pierre Sochala*, BRGM, France; Olivier P. Le Maitre, LIMSI-CNRS, France

#### 10:10-10:25 Multi-Objective Well Placement Optimization under Geological Uncertainty

*Yuqing Chang*, University of Oklahoma, USA; Zyed Bouzarkoun, Total, France; Deepak Devegowda, University of Oklahoma, USA

# 10:30-10:45 Uncertainty Propagation in Turbidity Currents Simulation

*Fernando A. Rochinha*, COPPE/Universidade Federal do Rio e Janeiro, Brazil; Gabriel Guerra, Federal University of Rio de Janerio, Brazil; Alvaro Coutinho, COPPE/ Universidade Federal do Rio e Janeiro, Brazil

#### 10:50-11:05 Investigation of Level Crossings in a Vertical Axis Wind Turbine (VAWT) using Probability Density Evolution Method (PDEM) Harshini Devathi and Sunetra Sarkar, Indian

Institute of Technology Madras, India

#### 11:10-11:25 Reliability-constrained Robust Design Optimization for Multireservoir River Systems

Veronika S. Vasylkivska, Nathan L. Gibson, Chris Hoyle, and Matthew McIntire, Oregon State University, USA

## Lunch Break 11:30 AM-1:00 PM

Attendees on their own

### Wednesday, April 2

### IP6 The Theory Behind Reduced Basis Methods

1:00 PM-1:45 PM

Room:Ballroom A/B/C - 2nd Floor

Chair: Clayton G. Webster, Oak Ridge National Laboratory, USA

Reduced basis methods are a popular numerical tool for solving parametric and stochastic partial differential equations. We will discuss the theory behind such methods in the case of elliptic parametric equations. The main question we will answer is when can we know a priori that these methods will perform better than simply calling on a standard Finite Element Solver or Adaptive Finite Element Solver. We shall see that this is related to the smoothness of the manifold of solutions and in particular to the Kolmogorov width of this manifold. We will also discuss when a particular implementation of reduced basis methods known as greedy algorithms will guarantee optimal performance.

Ronald DeVore Texas A&M University, USA

### Intermission

1:45 PM-2:00 PM

# MT6

### A Few Elements of Numerical Analysis for Elliptic PDEs with Random Coefficients of lognormal Type

2:00 PM-4:00 PM

Room:Ballroom A - 2nd Floor Chair: Julia Charrier, Aix-Marseille Université, France

In this minitutorial we will focus on the case of elliptic PDEs with lognormal coefficients, however most ideas are more general. Such coefficients raise several mathematical difficulties: they are neither uniformly bounded from above nor below, they may have low spatial regularity and have non-affine dependance on the random parameters. We will explain how to establish error estimates, by illustrating this in the cases of the Monte-Carlo method and the stochastic collocation method. This session is designed to complement MS69.

Julia Charrier, Aix-Marseille Université, France

### Wednesday, April 2

### MS60 Bayesian Analysis of Multifidelity Computer Codes

2:00 PM-4:00 PM

Room:Ballroom B - 2nd Floor

Complex computer codes are widely used in science and engineering to model physical phenomena. Furthermore, they can often be run at different levels of complexity and a hierarchy of levels of code can hence be obtained. The minisymposium deals with the Bayesian analysis of such computer codes using Cokriging models. In particular, recent advances in sequential design for improving the accuracy of a surrogate model, optimization methods, sensitivity analysis and calibration for multifidelity computer codes are presented.

Organizer: Loic Le Gratiet *EDF, France* 

Organizer: Claire Cannamela CEA, DAM, DIF-Bruyeres, France

2:00-2:25 Cokriging-Based Sequential Design for Multi-Fidelity Computer Codes

Loic Le Gratiet, EDF, France

### 2:30-2:55 A Bayesian Approach for Global Sensitivity Analysis of Multi-Fidelity Computer Codes

Claire Cannamela, CEA, DAM, DIF-Bruyeres, France

3:00-3:25 Addressing Multi-Fidelity Black Box Systems with Sequential Kriging Optimization Partition Envelope Method

Sayak RoyChowdh and Theodore T. Allen, Ohio State University, USA

### 3:30-3:55 Prediction and Computer Model Calibration Using Outputs From Multiple Computer Codes

Joslin Goh and Derek Bingham, Simon Fraser University, Canada

### Wednesday, April 2

# MS61

### Uncertainty Quantification and Reduction in Environmental Fluids -Part I of III

2:00 PM-4:00 PM

Room:Ballroom D - 2nd Floor

### For Part 2 see MS71

The purpose of this minisymposium is to report on recent advances in uncertainty quantification (UQ) methods with focus on environmental fluid dynamics applications, including, but not limited to, flow in porous media, hydrology, transport phenomena, atmospheric and oceanic modeling, climate, and extreme weather and coastal events. Relevant topics include forward propagation of uncertainties, inference of model parameters (inverse UQ) and data assimilation techniques. Also of relevance are statistical approaches to UQ based on Bayesian methods, the use of model reduction and emulators for efficient uncertainty propagation, Bayesian filtering methods, model parameter calibration techniques, and model error characterization.

Organizer: Ibrahim Hoteit King Abdullah University of Science & Technology (KAUST), Saudi Arabia

Organizer: Omar M. Knio Duke University, USA

Organizer: Mohamed Iskandarani University of Miami, USA

Organizer: Ahmed H. ElSheikh University of Texas at Austin, USA

2:00-2:25 Bayesian Approaches to the Analysis of Computer Model Output Mark Berliner, Ohio State University, USA

#### 2:30-2:55 Bayesian Prior Model Selection for Channelized Subsurface Flow Models

Ahmed H. ElSheikh, University of Texas at Austin, USA

### 3:00-3:25 Quantifying the Uncertainty in the Assessment of Climate Change Impact on Hydrologic Extremes using Hierarchical Bayesian Modeling

Hamid Moradkhani, Portland State University, USA

# 3:30-3:55 Displacement Assimilation when Features are Essential

Juan M. Restrepo, University of Arizona, USA

### Wednesday, April 2

# MS62

### Sensitivity Analysis and Data Inference in Highdimensional Stochastic Systems - Part I of II

2:00 PM-4:00 PM

Room:Ballroom E - 2nd Floor

### For Part 2 see MS72

This minisymposium will focus on mathematical and computational aspects of uncertainty quantification for highdimensional complex stochastic systems, also characterized by a potentially very high-dimensional parameter spaces. We discuss goal-oriented and information theory-based approaches, risk-sensitive measures, non-equilibrium statistical mechanics methods and applications to molecular and mesoscopic dynamics. Particular topics in the minisymposium include sensitivity analysis and data inference in molecular and other micro/meso-scale models, uncertainty and error quantification in processes that exhibit extreme events, complex stochastic systems with memory and correlated noise, and reliable model parameterizations and rational model selection.

Organizer: Markos A. Katsoulakis University of Massachusetts, Amherst, USA

Organizer: Petr Plechac University of Delaware, USA

Organizer: Jonathan Weare University of Chicago, USA

2:00-2:25 Renyi Entropy and Robustness in Rare Event Estimation Paul Dupuis, Brown University, USA

#### 2:30-2:55 Sensitivity Bounds and Error Estimates for Stochastic Models Paul Dupuis, Brown University, USA;

Markos A. Katsoulakis, University, USA, Massachusetts, Amherst, USA; Yannis Pantazis, University of Crete, Greece; *Petr Plechac*, University of Delaware, USA

#### 3:00-3:25 Goal-Oriented Sensitivity Analysis for lattice kinetic Monte Carlo Simulations

*Georgios Arampatzis*, University of Crete, Greece; Markos A. Katsoulakis, University of Massachusetts, Amherst, USA

#### 3:30-3:55 Irreversible Langevin Samplers: A Large Deviations Approach

Konstantinos Spiliopoulos, Boston University, USA

continued in next column

# MS63

### Active Subspace Methods for High-dimensional Approximation and Inverse Problems - Part II of II

2:00 PM-4:00 PM

Room:Ballroom F - 2nd Floor

### For Part 1 see MS54

Most methods for uncertainty quantification struggle with highdimensional parameter spaces due to the curse of dimensionality. Sensitivity analysis can reduce the dimension by identifying the important parameters, which enables UQ studies. However, most sensitivity analysis methods are restricted to the original parameters. Active subspace methods identify and exploit a set of directions---i.e., linear combinations of the original parameters---that are most important for approximation. This minisymposium explores the use of active subspace methods for (i) approximating functions of many parameters and (ii) solving inverse UQ problems with highdimensional inputs.

Organizer: Paul Constantine Colorado School of Mines, USA

### 2:00-2:25 Practical Considerations for Subspace Methods in Dakota

Brian M. Adams, Sandia National Laboratories, USA

### 2:30-2:55 Family-Direction-Selective Technique for Adaptive Multidimensional Hierarchical Sparse Grid Sampling

Miroslav Stoyanov, Oak Ridge National Laboratory, USA

### 3:00-3:25 On Directional Regression for Dimension Reduction

Bing Li, Pennsylvania State University, USA

#### 3:30-3:55 Active Subspace Identification in Surrogate Modeling Andrew Packard, University of California, Berkeley, USA

Wednesday, April 2

# MS64

### Advances in Optimal Experimental Design -Part II of IV

2:00 PM-4:00 PM

Room: Verelst Room - 2nd Floor

### For Part 1 see MS55 For Part 3 see MS74

The challenge of optimal information gathering---reflecting some end goal of inference, prediction, or control---pervades fields ranging from geophysics to systems biology to autonomy. Extending classical Bayesian experimental design methodologies to tackle problems of greater scale and dynamic complexity requires new algorithms and even new formulations. This minisymposium aims to cross-fertilize a wide variety of methodologies, where key challenges include: (1) design for ill-posed and large-scale inverse problems, nonlinear models, design in the presence of model error, and the estimation of information gain; and (2) optimal closed-loop (sequential) experimental design, harnessing rigorous approaches developed in multiple communities (e.g., controls, statistics, operations research).

Organizer: Xun Huan Massachusetts Institute of Technology, USA

Organizer: Youssef M. Marzouk Massachusetts Institute of Technology, USA

Organizer: Luis Tenorio Colorado School of Mines, USA

Organizer: Gabriel A. Terejanu University of Texas at Austin, USA

### 2:00-2:25 Sequential Experimental Design Using Dynamic Programming and Optimal Maps

*Xun Huan* and Youssef M. Marzouk, Massachusetts Institute of Technology, USA

### 2:30-2:55 Rapid Data Gathering using Mobile Robotic Vehicles

Sertac Karaman, Massachusetts Institute of Technology, USA

### 3:00-3:25 Optimal Information Trajectory Design for Dynamic State Estimation

*Nagavenkat Adurthi*, Reza Madankan, and Puneet Singla, State University of New York at Buffalo, USA

#### 3:30-3:55 A Framework for Sequential Experimental Design for Inverse Problems

Luis Tenorio, Colorado School of Mines, USA

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### MS65 Efficient Simulation of Rare Events - Part II of IV

### 2:00 PM-4:00 PM

Room: Percival Room - 2nd Floor

### For Part 1 see MS56 For Part 3 see MS75

Applications in materials science, theoretical chemistry, and atmosphere science call for efficient algorithms for simulation of rare events. The study of such events is crucial since they lead to important understanding of the system, for example, the failure of materials, the phase transition, chemical reaction, etc. Recent advances use ideas from importance sampling, large deviation theory, extreme value analysis, and uncertainty quantification. This minisymposium aims at bringing together experts and young researchers to discuss recent development and future directions. Topics include large deviation, importance sampling, discontinuity/edge detection, stochastic optimization/control, transition pathway, with applications in engineering, physics, biology and materials science.

### Organizer: Xiang Zhou City University of Hong Kong, Hong Kong

Organizer: Jianfeng Lu Duke University, USA

Organizer: Jingchen Liu Columbia University, USA

Organizer: Richard Archibald Oak Ridge National Laboratory, USA

Organizer: Guannan Zhang Oak Ridge National Laboratory, USA

#### 2:00-2:25 Hybrid Parallel Minimum Action Method and Its Applications

Xiaoliang Wan, Louisiana State University, USA

# 2:30-2:55 Simulating Rare Events in Groundwater Contaminant Transport

Jinglai Li, Shanghai Jiao Tong University, China; Xiang Zhou, City University of Hong Kong, Hong Kong

3:00-3:25 A Robust Approach to Computing Sensitivity to Serial Dependency in Input Processes *Henry Lam*, Boston University, USA

### 3:30-3:55 Large Deviations and Importance Sampling for Anomalous Shock Displacement

Tzu-wei Yang, University of Minnesota, USA

Wednesday, April 2

# MS66

### Spatial Aspects of Stochastic Sampling for Distributed Parameter Systems

### 2:00 PM-3:00 PM

### Room:Sloane Room - 2nd Floor

Stochastic sampling methods, although arguably the most direct and least intrusive means of incorporating parametric uncertainty into numerical simulations of partial differential equations with random inputs, may require a large number of sample simulations, each of which may need to be run at high levels of spatial fidelity to achieve a given level of accuracy. This minisymposium focuses on ways of improving the efficiency of sampling methods without compromising on their attractive features, through the systematic incorporation of spatial model attributes, such as parameter sensitivity or spatial refinement, or the recycling of deterministic solvers, into the sampling process.

Organizer: Hans-Werner Van Wyk Florida State University, USA

### 2:00-2:25 Multilevel Sparse Grid Methods for Pdes with Random Parameters

Hans-Werner Van Wyk, Florida State University, USA

2:30-2:55 Sensitivity Analysis and Uncertainty in Groundwater Flow Vitor Nunes, University of Texas at Dallas, USA

### Wednesday, April 2

## **MS67**

### Surrogate and Reduced Order Modeling for Statistical Inversion and Prediction -Part I of II

2:00 PM-4:00 PM

Room:Savannah Room - Lobby Level

### For Part 2 see MS77

An important and challenging task in computational simulation is the inference of model parameters from noisy and indirect data, along with using these parameter estimates for model predictions. In these processes, statistical methods, Bayesian methods in particular, play a fundamental role in modeling various information sources and quantifying uncertainty. Yet seemingly intractable computationally challenges arise when applying these methods to systems described by computationally intensive simulations. These challenges can be addressed with computationally efficient reduced-order or surrogate models. This minisymposium brings together researchers in various fields of surrogate modeling to present their current advances in methods for statistical inversion and prediction with expensive numerical simulation tools.

Organizer: Tiangang Cui Massachusetts Institute of Technology, USA

Organizer: Youssef M. Marzouk Massachusetts Institute of Technology, USA

Organizer: Karen E. Willcox Massachusetts Institute of Technology, USA

### 2:00-2:25 Ensemble Real-Time Control: Uncertainty, Data, Decisions.

Dennis McLaughlin and Binghuai Lin, Massachusetts Institute of Technology, USA

#### 2:30-2:55 Sequential Design with Mutual Information for Computer Experiments (MICE). Emulation of a Tsunami Simulator

Joakim Beck and Serge Guillas, University College London, United Kingdom

## **MS67**

Surrogate and Reduced Order Modeling for Statistical Inversion and Prediction -Part I of II

2:00 PM-4:00 PM

continued

#### 3:00-3:25 Approximate Marginalization of Source and Detector Coupling and Location Errors in Diffuse Optical Tomography

Meghdoot Mozumder and Tanja Tarvainen, University of Eastern Finland, Finland; Simon Arridge, University College London, United Kingdom; Jari Kaipio, University of Auckland, New Zealand; *Ville P. Kolehmainen*, University of Eastern Finland, Finland

#### 3:30-3:55 Data-Driven Model Reduction for the Bayesian Solution of Inverse Problems

*Tiangang Cui*, Youssef M. Marzouk, and Karen E. Willcox, Massachusetts Institute of Technology, USA

### Wednesday, April 2

## **MS68**

UQ for Inverse Problems: Data Assimilation, Parameter Estimation, and Sampling -Part II of III

2:00 PM-4:00 PM

Room:Plimsoll - Lobby Level

#### For Part 1 see MS59 For Part 3 see MS78

In inverse problems, parameters in a physical model are estimated from indirect measurements. Due to modeling errors and random noise in the measurement process, any estimator of the unknown parameters is a random quantity, and hence quantifying uncertainty in the estimator is an important task. In this minisymposium, the talks focus on techniques for uncertainty quantification in inverse problems. The topics considered include classical applications in inverse problems, such as x-ray radiography and electrical impedance tomography; parameter estimation for ODE models; data assimilation for weather prediction; and Monte Carlo sampling methods.

Organizer: Johnathan M. Bardsley University of Montana, USA

### 2:00-2:25 Estimating Baye's Factors of Approximate Numerical and Theoretical Posteriors for Optimal Precision Evaluation in the Bayesian Analysis of ODEs

J. Andrés Christen, CIMAT, Mexico

2:30-2:55 Matrix Splittings As Generalized Langevin and Hamiltonian Proposals for MCMC *Richard A. Norton* and Colin Fox, University of Otago, New Zealand

3:00-3:25 Using Polynomials to Sample from Large Gaussians Used to Model 3-D Confocal Microscope Images of Biofilms

Albert Parker, Montana State University, USA

3:30-3:55 Inference with Continuous-Time Markov Jump Processes Via the Van Kampen Expansion

Marcos A. Capistran, CIMAT, Mexico

### Wednesday, April 2

# CP14 Fluid Mechanics

2:00 PM-4:00 PM

Room: Vernon Room - 2nd Floor

Chair: Jaideep Ray, Sandia National Laboratories, USA

#### 2:00-2:15 Non-Intrusive Polynomial Chaos Method in Hypersonic Scramjet Intake Flow

*Sarah Frauholz*, Birgit Reinartz, Sigfried Müller, and Marek Behr, RWTH Aachen University, Germany

#### 2:20-2:35 Deterministic Sampling for Uncertainty Quantification in Computational Fluid Dynamics

Peter Hedberg, Swedish Radiation Safety Authority, Sweden

#### 2:40-2:55 Numerical Evaluation of a Parallel Stochastic Galerkin Solver for the Steady Incompressible Navier-Stokes Equations with Random Parameters

Michael Schick and Vincent Heuveline, Heidelberg University, Germany

#### 3:00-3:15 Reconstructing Incompressible Flow Fields by Using a Physics-Based Covariance Model for Gaussian Processes

Iliass Azijli, Richard Dwight, and Hester Bijl, Delft University of Technology, Netherlands

# 3:20-3:35 Tuning a RANS k-e Model for Jet-in-Crossflow Simulations

Sophia Lefantzi, *Jaideep Ray*, Srinivasan Arunajatesan, and Lawrence Dechant, Sandia National Laboratories, USA

### 3:40-3:55 Incompressible Navier-Stokes Equations with Stochastic Viscosity

Mass Per Pettersson, Stanford University, USA; Alireza Doostan, University of Colorado Boulder, USA; Jan Nordström, Linköping University, Sweden

### Coffee Break



Room:Regency Foyer and Promenade - 2nd Floor

4:00 PM-4:30 PM

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Wednesday, April 2

# **MS69**

### PDEs with Random Coefficients of lognormal Type and Applications to Subsurface Flow

### 4:30 PM-6:30 PM

Room:Ballroom A - 2nd Floor

In this minisymposium, we would like to focus on numerical methods for PDEs with random coefficients that are neither uniformly bounded from above nor below and that have possibly low regularity. An important case of such a coefficient is a lognormal coefficient, which is widely used in hydrogeology and petroleum engineering to model the uncertainty in the permeability field in subsurface flow. This has important applications in radioactive waste management, in CO2-sequestration and in the optimisation of oil/gas reservoir exploitation. The mini-symposium will gather both theoretical as well as application talks on this topic, focussing on different approaches to deal with the above mentioned difficulties. This session is designed to complement MT6.

Organizer: Julia Charrier Aix-Marseille Université, France

Organizer: Robert Scheichl University of Bath, United Kingdom

4:30-4:55 Numerical Analysis of the Advection-Diffusion of a Solute in Porous Media with Uncertainty

Julia Charrier, Aix-Marseille Université, France

#### 5:00-5:25 Computation of Macro Spreading in 3D Porous Media with Uncertain Data

Anthony Beaudoin, Université de Poitiers, France; Jean Raynald de Dreuzy, CNRS, Université de Rennes 1, France; *Jocelyne Erhel* and Mestapha Oumouni, INRIA-Rennes, France

### 5:30-5:55 Multilevel Monte Carlo Methods for Uncertainty Quantification in Subsurface Flow

Aretha L. Teckentrup, Florida State University, USA; Julia Charrier, Aix-Marseille Université, France; Andrew Cliffe, University of Nottingham, United Kingdom; Mike Giles, University of Oxford, United Kingdom; Robert Scheichl, University of Bath, United Kingdom

### 6:00-6:25 Stochastic Collocation for Elliptic Pdes with Random Data - The Lognormal Case

Oliver G. Ernst and Björn Sprungk, TU Chemnitz, Germany

### Wednesday, April 2

# **MS70**

### Numerical Methods for Uncertainty Quantification of Coupled Problems -Part II of V

4:30 PM-6:30 PM

Room:Ballroom B - 2nd Floor

### For Part 1 see MS51 For Part 3 see MS79

Accurate prediction of many engineering systems often requires simulations of tightly coupled and interacting phenomena with multiple physics or domains and at multiple scales. When uncertainties are present, the UQ of such coupled systems is challenged by two difficulties. First, the presence of independent uncertainty sources within different physics/scale models results in a combined highdimensional stochastic space which may not be amenable to fast computation using standard approaches. Second, single physics/scale solvers are separate modules that may not have access to detailed information from one another. This minisymposium invites contributions that discuss the above challenges and provide novel solution techniques.

Organizer: Dongbin Xiu University of Utah, USA

Organizer: Alireza Doostan University of Colorado Boulder, USA

4:30-4:55 Multi-resolution Method for Emulator Construction

Abani K. Patra and *Elena Stefanescu*, State University of New York, Buffalo, USA

### 5:00-5:25 Active Subspace Sensitivity Analysis for Fully Coupled Systems with Independent Parameters

Paul Constantine, Colorado School of Mines, USA

5:30-5:55 A Domain Decomposition Approach for Uncertainty Analysis *Qifeng Liao* and Karen E. Willcox, Massachusetts Institute of Technology, USA

6:00-6:25 Not available at time of publication

Yanzhao Cao, Auburn University, USA

2014 SIAM Conference on Uncertainty Quantification

Wednesday, April 2

## **MS71**

### Uncertainty Quantification and Reduction in Environmental Fluids -Part II of III

4:30 PM-6:30 PM

Room:Ballroom D - 2nd Floor

### For Part 1 see MS61 For Part 3 see MS80

The purpose of this minisymposium is to report on recent advances in uncertainty quantification (UO) methods with focus on environmental fluid dynamics applications, including, but not limited to, flow in porous media, hydrology, transport phenomena, atmospheric and oceanic modeling, climate, and extreme weather and coastal events. Relevant topics include forward propagation of uncertainties, inference of model parameters (inverse UQ) and data assimilation techniques. Also of relevance are statistical approaches to UQ based on Bayesian methods, the use of model reduction and emulators for efficient uncertainty propagation, Bayesian filtering methods, model parameter calibration techniques, and model error characterization.

Organizer: Ibrahim Hoteit King Abdullah University of Science & Technology (KAUST), Saudi Arabia

Organizer: Omar M. Knio Duke University, USA

Organizer: Mohamed Iskandarani University of Miami, USA

Organizer: Ahmed H. ElSheikh University of Texas at Austin, USA

### 4:30-4:55 Mitigating Observation Error Undersamling in the Stochastic EnKF

*Ibrahim Hoteit*, King Abdullah University of Science & Technology (KAUST), Saudi Arabia

### 5:00-5:25 A Diagnostic Approach to Model Evaluation: Approximate Bayesian Computation

Jasper Vrugt and Mojtaba Sadegh, University of California, Irvine, USA

### 5:30-5:55 Bayesian History Matching and Uncertainty Quantification under Sparse Priors: A Randomized Maximum Likelihood Approach

Benham Jafarpour, University of Southern California, USA

### 6:00-6:25 Pragmatic Aspects of Quadrature for Propagating Uncertainty

Carlisle Thacker, Rosenstiel School of Marine and Atmospheric Science, USA Wednesday, April 2

### MS72 Sensitivity Analysis and Data Inference in Highdimensional Stochastic

Systems - Part II of II

4:30 PM-6:30 PM

Room:Ballroom E - 2nd Floor

### For Part 1 see MS62

This minisymposium will focus on mathematical and computational aspects of uncertainty quantification for highdimensional complex stochastic systems, also characterized by a potentially very high-dimensional parameter spaces. We discuss goal-oriented and information theory-based approaches, risk-sensitive measures, non-equilibrium statistical mechanics methods and applications to molecular and mesoscopic dynamics. Particular topics in the minisymposium include sensitivity analysis and data inference in molecular and other micro/meso-scale models, uncertainty and error quantification in processes that exhibit extreme events, complex stochastic systems with memory and correlated noise, and reliable model parameterizations and rational model selection.

Organizer: Markos A. Katsoulakis University of Massachusetts, Amherst, USA

Organizer: Petr Plechac University of Delaware, USA

Organizer: Jonathan Weare University of Chicago, USA

4:30-4:55 Geometric Methods for the Approximation of High-dimensional Dynamical Systems

Mauro Maggioni, Duke University, USA

5:00-5:25 PDF Method for Langevin Dynamics Driven by Colored Noise Peng Wang, Pacific Northwest National Laboratory, USA

5:30-5:55 Modelling and Estimating Multivariate Jump Diffusion Models Omiros Papaspiliopoulos, Universitat Pompeu Fabra, Spain

6:00-6:25 Stratification of Markov Processes for Rare Event Simulation Jonathan Weare, University of Chicago, USA

## **MS73**

### **Theoretical and Numerical** Analysis for Forward-**Backward Stochastic Differential Equations and Stochastic Optimal Control** - Part I of IV

4:30 PM-6:30 PM

Room:Ballroom F - 2nd Floor

### For Part 2 see MS82

Forward-Backward SDEs (FBSDEs) have been widely studied in connection with partial differential equations, stochastic optimal control, nonlinear filtering and mathematical finance. The theoretical and numerical analyses of FBSDEs are more complicated than that of classical SDEs, so that there are many interesting and challenging open problems in this area. The minisymposium aims at exploring efforts related to theoretical and numerical analysis for FBSDEs including, but not limited to, BSDEs/FBSDEs theories, nonlinear expectations, FBDSDEs and nonlinear filtering, FBSDE-based stochastic optimal control, high-order numerical methods for FBSDEs, numerical solution for high-dimensional FBSDEs.

Shandong University, China

Organizer: Weidong Zhao Shandong University, China

Organizer: Guannan Zhang Oak Ridge National Laboratory, USA

#### 4:30-4:55 Efficient Empirical **Regression Methods for Solving** Forward-Backward Stochastic **Differential Equations**

Gobet Emmanuel and Plamen Turkedjiev, Ecole Polytechnique, France

### 5:00-5:25 A Fundamental **Convergence Theorem of Numerical** Methods for BSDEs

Jialin Hong, Chinese Academy of Sciences, China

Organizer: Zhen Wu

5:30-5:55 A Primal-Dual Algorithm for Backward Stochastic Differential **Equations** 

Christian Bender and Nikolaus Schweizer, Universität des Saarlandes, Germany; Jia Zhuo, University of Southern California, USA

6:00-6:25 A New Kind of Multistep Method for Forward Backward **Stochastic Differential Equations** Weidong Zhao, Shandong University, China Wednesday, April 2

# **MS74**

### Advances in Optimal **Experimental Design -**Part III of IV

4:30 PM-6:00 PM

Room: Verelst Room - 2nd Floor

#### For Part 2 see MS64 For Part 4 see MS83

The challenge of optimal information gathering---reflecting some end goal of inference, prediction, or control---pervades fields ranging from geophysics to systems biology to autonomy. Extending classical Bayesian experimental design methodologies to tackle problems of greater scale and dynamic complexity requires new algorithms and even new formulations. This minisymposium aims to cross-fertilize a wide variety of methodologies, where key challenges include: (1) design for ill-posed and largescale inverse problems, nonlinear models, design in the presence of model error, and the estimation of information gain; and (2) optimal closed-loop (sequential) experimental design, harnessing rigorous approaches developed in multiple communities (e.g., controls, statistics, operations research).

Organizer: Xun Huan Massachusetts Institute of Technology, USA

Organizer: Youssef M. Marzouk Massachusetts Institute of Technology, USA

Organizer: Luis Tenorio Colorado School of Mines, USA

Organizer: Gabriel A. Terejanu University of Texas at Austin, USA

### 4:30-4:55 Bayesian Subgroup Finding by Stochastic Optimization

Peter Mueller, University of Texas at Austin, USA; Riten Mitra, University of Louisville, USA; Lurdes Inoue, University of Washington, USA

#### 5:00-5:25 Two-Stage Predictor Design in **High Dimensions**

Hamed Firouzi, University of Michigan, USA; Bala Rajaratnam, Stanford University, USA; Alfred O. Hero, The University of Michigan, Ann Arbor, USA

#### 5:30-5:55 Cross Validation for **Uncertainty Quantification Using Sparse** Grids

Frederick Boehm and Peter Qian, University of Wisconsin, Madison, USA

continued in next column

### MS75 Efficient Simulation of Rare Events - Part III of Part IV

4:30 PM-6:30 PM

Room: Percival Room - 2nd Floor

### For Part 2 see MS65 For Part 4 see MS84

Applications in materials science, theoretical chemistry, and atmosphere science call for efficient algorithms for simulation of rare events. The study of such events is crucial since they lead to important understanding of the system, for example, the failure of materials, the phase transition, chemical reaction, etc. Recent advances use ideas from importance sampling, large deviation theory, extreme value analysis, and uncertainty quantification. This minisymposium aims at bringing together experts and young researchers to discuss recent development and future directions. Topics include large deviation, importance sampling, discontinuity/edge detection, stochastic optimization/control, transition pathway, with applications in engineering, physics, biology and materials science.

Organizer: Xiang Zhou City University of Hong Kong, Hong Kong

Organizer: Jianfeng Lu Duke University, USA

Organizer: Jingchen Liu Columbia University, USA

Organizer: Richard Archibald Oak Ridge National Laboratory, USA

Organizer: Guannan Zhang Oak Ridge National Laboratory, USA

#### 4:30-4:55 Analysis of the Lennard-Jones-38 Stochastic Network at Temperatures from Zero to the Melting Point

Maria K. Cameron, New York University, USA

5:00-5:25 Sampling Saddle Point on the Free Energy Surface of Complex Systems

Amit Samanta, Princeton University, USA

### 5:30-5:55 Quantification of Extremely High Excursion Solution of Elliptic Equation with Random Coefficients

*Xiang Zhou*, City University of Hong Kong, Hong Kong; Jianfeng Lu, Duke University, USA; Jingchen Liu, Columbia University, USA

### 6:00-6:25 Rare Event Simulation for Reflecting Brownian Motion via Splitting Algorithm

Kevin Leder, University of Minnesota, USA; *Xin Liu*, Clemson University, USA Wednesday, April 2

### MS76 Statistical Methods for Model Calibration and Uncertainty Quantification

4:30 PM-6:30 PM

### Room:Sloane Room - 2nd Floor

Scientific and engineering model development involves several simplifying assumptions for the purpose of mathematical tractability which are often not realistic in practice. This leads to biases in the model predictions. Bayesian methods using Gaussian process modeling for simultaneous model calibration and bias correction are widely used for this purpose because they can easily incorporate the various sources of uncertainty including the errors in the model approximation. This minisymposium will contain four talks encompassing the theoretical and practical aspects of the methodology.

Organizer: V. Roshan Joseph Georgia Institute of Technology, USA

4:30-4:55 A Theoretical Framework for Calibration in Computer Models: Parametrization, Estimation and Convergence Properties *Jeff Wu*, Georgia Institute of Technology, USA

#### 5:00-5:25 A Multiple-Response Approach to Improving Identifiability in Model Calibration and Bias Correction

Zhen Jiang, Wei Chen, and Dan Apley, Northwestern University, USA

### 5:30-5:55 Connecting Model-Based Predictions to Reality

David Higdon, Los Alamos National Laboratory, USA

### 6:00-6:25 Sequential Strategies Based on Bayesian Uncertainty Quantification for Linear Sparse Surrogate Models

Ray-Bing Chen, National Cheng Kung University, Taiwan; Weichung Wang, National Taiwan University, Taiwan; Jeff Wu, Georgia Institute of Technology, USA

## **MS77**

### Surrogate and Reduced Order Modeling for Statistical Inversion and Prediction - Part II of II

### 4:30 PM-6:30 PM

Room:Savannah Room - Lobby Level

### For Part 1 see MS67

An important and challenging task in computational simulation is the inference of model parameters from noisy and indirect data, along with using these parameter estimates for model predictions. In these processes, statistical methods, Bayesian methods in particular, play a fundamental role in modeling various information sources and quantifying uncertainty. Yet seemingly intractable computationally challenges arise when applying these methods to systems described by computationally intensive simulations. These challenges can be addressed with computationally efficient reduced-order or surrogate models. This minisymposium brings together researchers in various fields of surrogate modeling to present their current advances in methods for statistical inversion and prediction with expensive numerical simulation tools.

Organizer: Tiangang Cui Massachusetts Institute of Technology, USA

Organizer: Youssef M. Marzouk Massachusetts Institute of Technology, USA

Organizer: Karen E. Willcox Massachusetts Institute of Technology, USA

#### 4:30-4:55 Stochastic DtN Map, Electrical Impedance Tomography and Boundary Truncation

Jari Kaipio and Paul Hadwin, University of Auckland, New Zealand; Janne Huttunen, University of Eastern Finland, Finland; Daniela Calvetti and Erkki Somersalo, Case Western Reserve University, USA; Joe Volzer and Debra McGivney, Case Western Reserve University, USA

### 5:00-5:25 A Local Approximation Framework for Accelerating MCMC with Computationally Intensive Models

Patrick R. Conrad, Massachusetts Institute of Technology, USA; Natesh Pillai, Harvard University, USA; Youssef M. Marzouk, Massachusetts Institute of Technology, USA

### 5:30-5:55 Electrical Impedance Tomography Imaging with Reducedorder Model based on Proper Orthogonal Decomposition

Aku Seppanen and Antti Lipponen, University of Eastern Finland, Finland; Jari Kaipio, University of Auckland, New Zealand

# 6:00-6:25 Methods for Data Reduction in Uncertainty Quantification

Laura Swiler, Sandia National Laboratories, USA

### Wednesday, April 2

# **MS78**

### UQ for Inverse Problems: Data Assimilation, Parameter Estimation, and Sampling -Part III of III

4:30 PM-6:30 PM

Room:Plimsoll - Lobby Level

### For Part 2 see MS68

In inverse problems, parameters in a physical model are estimated from indirect measurements. Due to modeling errors and random noise in the measurement process, any estimator of the unknown parameters is a random quantity, and hence quantifying uncertainty in the estimator is an important task. In this minisymposium, the talks focus on techniques for uncertainty quantification in inverse problems. The topics considered include classical applications in inverse problems, such as x-ray radiography and electrical impedance tomography; parameter estimation for ODE models; data assimilation for weather prediction; and Monte Carlo sampling methods.

Organizer: Johnathan M. Bardsley University of Montana, USA

#### 4:30-4:55 Randomize-Then-Optimize: a Method for Sampling from Posterior Distributions in Nonlinear Inverse Problems

Johnathan M. Bardsley, University of Montana, USA; Antti Solonen, Lappeenranta University of Technology, Finland; Aku Seppanen, University of Eastern Finland, Finland; Heikki Haario, Lappeenranta University of Technology, Finland; Marko Laine, Finnish Meteorological Institute, Helsinki, Finland; Jari P. Kaipio, University of Eastern Finland, Finland and University of Auckland, New Zealand

### 5:00-5:25 Parameter Estimation in Large Scale State Space Models Using Ensembles of Model Runs

Marko Laine and Pirkka Ollinaho, Finnish Meteorological Institute, Helsinki, Finland; Heikki Järvinen, University of Helsinki, Finland; Antti Solonen, Lappeenranta University of Technology, Finland

## **MS78**

### UQ for Inverse Problems: Data Assimilation, Parameter Estimation, and Sampling - Part III of III

4:30 PM-6:30 PM

continued

### 5:30-5:55 UQ with Edge Location for Quantitative Radiography

Michael J. Fowler, Clarkson University, USA; Marylesa Howard and Aaron B. Luttman, National Security Technologies, LLC, USA

### 6:00-6:25 Point Spread Reconstruction in Radiography

*Kevin Joyce* and Johnathan M. Bardsley, University of Montana, USA

### Wednesday, April 2

## CP15

### Sampling 4:30 PM-6:10 PM

Room:Vernon Room - 2nd Floor

Chair: Fabrice Gamboa, University of Toulouse, France

### 4:30-4:45 Quasi Monte Carlo Sample Selection for Dependent Uncertainty Spaces

Jason W. Adaska and Gareth Middleton, Numerica, USA

### 4:50-5:05 Sharp Asymptotic for the Pick Freeze Estimation of the Sobol Indices

*Fabrice Gamboa*, University of Toulouse, France

### 5:10-5:25 Deterministic Sampling for Efficient and Accurate Quantification of Uncertainty

Peter J. Hessling, SP Technical Research Institute of Sweden, Sweden

### 5:30-5:45 Estimation of the Sobol Indices in a Linear Functional Multidimensional Model

Agnès Lagnoux, Universite de Toulouse, France

### 5:50-6:05 Randomized Pick-Freeze for Sparse Estimation of Sobol Indices in High Dimension

*Alexandre Janon* and Yohann De Castro, Université Paris-Sud, France; Fabrice Gamboa, University of Toulouse, France

## Thursday, April 3

## **Registration** 7:30 AM-5:00 PM

Room:Registration Booth - 2nd Floor

### **Closing Remarks**

8:10 AM-8:15 AM Room:Ballroom A/B/C - 2nd Floor

## IP7 Uncertainties Without the Rev. Thomas Bayes

8:15 AM-9:00 AM

Room:Ballroom A/B/C - 2nd Floor

Chair: Marcia McNutt, Science Magazine, American Association for the Advancement of Science, USA

Inverse problems in geophysics always fail to have unique solutions because of incompleteness of the measurements. None-the-less, it is often possible to obtain valuable insights by formulating a suitable optimization problem and thereby bounding some useful property, such as the average value in a region. Examples will be given from planetary science, bore-hole well logging of NRM data, and electromagnetic sounding.

Robert Parker University of California, San Diego, USA

### **Coffee Break**



Room:Regency Foyer and Promenade - 2nd Floor

9:00 AM-9:30 AM

### MT7 Numerical Analysis for PDEs with Random Inputs

9:30 AM-11:30 AM

Room:Ballroom A - 2nd Floor

Chair: Raul F. Tempone, King Abdullah University of Science & Technology (KAUST), Saudi Arabia

We provide an introduction to numerical methods for Uncertainty Quantification. We start by discussing data parametrization and then we study the implementation and convergence of several methods for forward propagation. To this end, we begin with Monte Carlo and Multi level Monte Carlo sampling and then show the use how to exploit higher solution regularity within  $L^2$  projection and discrete  $L^2$  projection methods. Throughout the presentation, numerical examples provide insight into the theory.

Fabio Nobile, EPFL, France; *Raul F. Tempone*, King Abdullah University of Science & Technology (KAUST), Saudi Arabia

## Thursday, April 3

## **MS79**

Numerical Methods for Uncertainty Quantification of Coupled Problems -Part III of V

9:30 AM-11:30 AM

Room:Ballroom B - 2nd Floor

### For Part 2 see MS70 For Part 4 see MS89

Accurate prediction of many engineering systems often requires simulations of tightly coupled and interacting phenomena with multiple physics or domains and at multiple scales. When uncertainties are present, the UO of such coupled systems is challenged by two difficulties. First, the presence of independent uncertainty sources within different physics/ scale models results in a combined high- dimensional stochastic space which may not be amenable to fast computation using standard approaches. Second, single physics/scale solvers are separate modules that may not have access to detailed information from one another. This minisymposium invites contributions that discuss the above challenges and provide novel solution techniques.

Organizer: Alireza Doostan University of Colorado Boulder, USA

Organizer: Dongbin Xiu University of Utah, USA

9:30-9:55 Bayesian Brittleness

Houman Owhadi, California Institute of Technology, USA; *Tim Sullivan*, University of Warwick, United Kingdom; Clint Scovel, Los Alamos National Laboratory, USA

# 10:00-10:25 Stochastic Modeling of the Land-Air Interface in the Cesm

Matthew Plumlee, Georgia Institute of Technology, USA; Richard Archibald and Roisin T. Langan, Oak Ridge National Laboratory, USA

#### 10:30-10:55 Stochastic Airfoil Model with the Joint Response-Excitation Pdf Approach

*Heyrim Cho*, Daniele Venturi, and George E. Karniadakis, Brown University, USA

#### 11:00-11:25 An Adaptive ANOVAbased Data-driven Stochastic Method for Elliptic PDE with Random Coecients *Guang Lin*, Pacific Northwest National

Laboratory, USA; Zhiwen Zhang, California Institute of Technology, USA; Xin Hu, CGGVeritas, Brazil; Pengchong Yan and Tom Hou, California Institute of Technology, USA

## **MS80**

### Uncertainty Quantification and Reduction in Environmental Fluids -Part III of III

9:30 AM-11:30 AM

Room:Ballroom D - 2nd Floor

### For Part 2 see MS71

The purpose of this minisymposium is to report on recent advances in uncertainty quantification (UQ) methods with focus on environmental fluid dynamics applications, including, but not limited to, flow in porous media, hydrology, transport phenomena, atmospheric and oceanic modeling, climate, and extreme weather and coastal events. Relevant topics include forward propagation of uncertainties, inference of model parameters (inverse UQ) and data assimilation techniques. Also of relevance are statistical approaches to UQ based on Bayesian methods, the use of model reduction and emulators for efficient uncertainty propagation, Bayesian filtering methods, model parameter calibration techniques, and model error characterization.

Organizer: Ibrahim Hoteit King Abdullah University of Science & Technology (KAUST), Saudi Arabia

Organizer: Omar M. Knio Duke University, USA

Organizer: Mohamed Iskandarani University of Miami, USA

Organizer: Ahmed H. ElSheikh University of Texas at Austin, USA

### 9:30-9:55 Towards Non-Gaussian Nonlinear Smoothing and Adaptive Sampling

Pierre Lermusiaux and Tapovan Lolla, Massachusetts Institute of Technology, USA

### 10:00-10:25 An Ensemble Kalman Filter for Statistical Estimation of Physics Constrained Nonlinear Regression Models

John Harlim, Pennsylvania State University, USA; Adam Mahdi, North Carolina State University, USA; Andrew Majda, Courant Institute of Mathematical Sciences, New York University, USA

### 10:30-10:55 Data Assimilation and Uncertainty Quantification of Co2 Sequestration Process Using Both Fluid Flow and Geo-Mechanical Observation

*Reza Tavakoli*, Benjamin Ganis, and Mary F. Wheeler, The University of Texas at Austin, USA

### 11:00-11:25 An MCMC Algorithm for Parameter Estimation of Partially Observed Signals with Intermittent Instability

Nan Chen and Dimitris Giannakis, New York University, USA; Radu Herbei, Ohio State University, USA; Andrew Majda, Courant Institute of Mathematical Sciences, New York University, USA

### Thursday, April 3

## **MS81** HPC Meets UQ - Part I of II 9:30 AM-11:00 AM

Room:Ballroom E - 2nd Floor

### For Part 2 see MS99

Uncertainty quantification increases the insight that can be gained through simulations in CSE at the price of significantly increased complexity. Besides the need for sophisticated mathematical approaches, performing UQ typically multiplies the computational costs by several orders of magnitude compared to the single deterministic simulations. Thus, high-performance computing aspects are ubiquitous in UQ across various disciplines and applications. The combination of these two fields is highly relevant and challenging, in particular with respect to the paradigm shifts in HPC in the era of massively parallel computing. This minisymposium is organised in collaboration with the German Priority Programme SPPEXA "Software for Exascale Computing" and addresses aspects of HPC in UQ.

Organizer: Tobias Neckel TU München, Germany

Organizer: George Biros University of Texas at Austin, USA

Organizer: Dirk Pflüger Universität Stuttgart, Germany

# 9:30-9:55 Not available at time of publication

George Biros, University of Texas at Austin, USA

### 10:00-10:25 Massively Parallel PDE Solvers for Uncertainty Quantification

Ulrich J. Ruede, University of Erlangen-Nuremberg, Germany; Björn Gmeiner, Universität Erlangen, Germany; Martin Bauer, University of Erlangen-Nuremberg, Germany

10:30-10:55 Bayesian Pca for High Dimensional Random Fields

Kenny Chowdhary and Habib N. Najm, Sandia National Laboratories, USA

## **MS82**

### Theoretical and Numerical Analysis for Forward-Backward Stochastic Differential Equations and Stochastic Optimal Control -Part II of IV

9:30 AM-11:30 AM

Room:Ballroom F - 2nd Floor

### For Part 1 see MS73 For Part 3 see MS92

Forward-Backward SDEs (FBSDEs) have been widely studied in connection with partial differential equations, stochastic optimal control, nonlinear filtering and mathematical finance. The theoretical and numerical analyses of FBSDEs are more complicated than that of classical SDEs, so that there are many interesting and challenging open problems in this area. The minisymposium aims at exploring efforts related to theoretical and numerical analysis for FBSDEs including, but not limited to, BSDEs/FBSDEs theories, nonlinear expectations, FBDSDEs and nonlinear filtering, FBSDE-based stochastic optimal control, high-order numerical methods for FBSDEs. numerical solution for high-dimensional FBSDEs.

Organizer: Zhen Wu Shandong University, China

Organizer: Weidong Zhao Shandong University, China

Organizer: Guannan Zhang Oak Ridge National Laboratory, USA

9:30-9:55 Second-Order Bsdes with General Reflection and Game Options under Uncertainty Anis Matoussi, University of Maine, USA

10:00-10:25 Approximate FBSDE Using Branching Particle Systems *Jie Xiong*, University of Tennessee, USA

# 10:30-10:55 Interacting Particle System and Optimal Stopping

*Peng Hu*, University of Oxford, United Kingdom; Nadia Oudjane, EDF, France; Pierre Del Moral, INRIA and University of Bordeaux, France

### 11:00-11:25 BSDEs with Markov Chains: Two-Time-Scale and Weak Convergence

Zhen Wu, Shandong University, China

Thursday, April 3

# MS83

### Advances in Optimal Experimental Design -Part IV of IV

9:30 AM-11:30 AM

Room: Verelst Room - 2nd Floor

### For Part 3 see MS74

The challenge of optimal information gathering---reflecting some end goal of inference, prediction, or control---pervades fields ranging from geophysics to systems biology to autonomy. Extending classical Bayesian experimental design methodologies to tackle problems of greater scale and dynamic complexity requires new algorithms and even new formulations. This minisymposium aims to cross-fertilize a wide variety of methodologies, where key challenges include: (1) design for ill- posed and large-scale inverse problems, nonlinear models, design in the presence of model error, and the estimation of information gain; and (2) optimal closed-loop (sequential) experimental design, harnessing rigorous approaches developed in multiple communities (e.g., controls, statistics, operations research).

Organizer: Xun Huan Massachusetts Institute of Technology, USA

Organizer: Youssef M. Marzouk Massachusetts Institute of Technology, USA

Organizer: Luis Tenorio Colorado School of Mines, USA

Organizer: Gabriel A. Terejanu University of Texas at Austin, USA

9:30-9:55 Design of Data Collection When Standard DoE Is Not Available *Heikki Haario*, Lappeenranta University of Technology, Finland

### 10:00-10:25 A Scalable MAP-Based Algorithm for Optimal Experimental Design for Large-Scale Bayesian Inverse Problems

Alen Alexanderian, Noemi Petra, Georg Stadler, and Omar Ghattas, University of Texas at Austin, USA

## MS83

### Advances in Optimal Experimental Design -Part IV of IV

9:30 AM-11:30 AM

continued

#### 10:30-10:55 Fast Bayesian Optimal Design

*Quan Long*, King Abdullah University of Science & Technology (KAUST), Saudi Arabia; Marco Scavino, Universidad de la República, Uruguay; Raul F. Tempone, King Abdullah University of Science & Technology (KAUST), Saudi Arabia; Suojin Wang, Texas A&M University, USA

#### 11:00-11:25 A Matrix Free Approach for Optimal Experimental Design for Inverse Problems

Thomas Carraro and Maria Woydich, Universität Heidelberg, Germany

### Thursday, April 3

### MS84 Efficient Simulation of Rare Events - Part IV of IV

9:30 AM-11:30 AM

Room:Percival Room - 2nd Floor

### For Part 3 see MS75

Applications in materials science, theoretical chemistry, and atmosphere science call for efficient algorithms for simulation of rare events. The study of such events is crucial since they lead to important understanding of the system, for example, the failure of materials, the phase transition, chemical reaction, etc. Recent advances use ideas from importance sampling, large deviation theory, extreme value analysis, and uncertainty quantification. This minisymposium aims at bringing together experts and young researchers to discuss recent development and future directions. Topics include large deviation, importance sampling, discontinuity/edge detection, stochastic optimization/control, transition pathway, with applications in engineering, physics, biology and materials science.

Organizer: Xiang Zhou City University of Hong Kong, Hong Kong

Organizer: Jianfeng Lu Duke University, USA

Organizer: Jingchen Liu Columbia University, USA

Organizer: Richard Archibald Oak Ridge National Laboratory, USA

Organizer: Guannan Zhang Oak Ridge National Laboratory, USA

9:30-9:55 A New Class of Stable Processes: Modeling and Bayesian Computation

Rui Tuo, Oak Ridge National Laboratory, USA

#### 10:00-10:25 Robust Bounds on Risk-Sensitive Functionals Via Renyi Divergence with Applications to Rare Events

Kenny Chowdhary, Sandia National Laboratories, USA; Rami Atar, Technion, Haifa, Israel; Paul Dupuis, Brown University, USA

### 10:30-10:55 Bayesian Discontinuity Detection and Surrogate Construction for Complex Computer Models

*Cosmin Safta*, Khachik Sargsyan, Bert J. Debusschere, and Habib N. Najm, Sandia National Laboratories, USA

### 11:00-11:25 Statistical Analysis of Extremes and Tail Dependence

Dan Cooley, Colorado State University, USA; Grant B. Weller, Carnegie Mellon University, USA; *Brook Russell*, Colorado State University, USA

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### Thursday, April 3

## **MS86**

### Stochastic Models, UQ and Inversion of Large-scale High-dimensional Complex Systems - Part I of II

### 9:30 AM-11:30 AM

Room:Sloane Room - 2nd Floor

### For Part 2 see MS93

Our aim is to use accurate computational simulations to predict the behavior of complex systems. Many stochastic algorithms and techniques have been developed. The explosion in computational effort associated with the large number of random dimensions is often prohibitive, even for modern supercomputers. As such, advanced stochastic approximation techniques are necessary to minimize the complexity of mathematical models and make numerical solutions feasible. This minisymposium will explore recent advances in numerical algorithms and applications for uncertainty quantification, model reduction, and stochastic inversion in large-scale highdimensional complex systems.

Organizer: Guang Lin Pacific Northwest National Laboratory, USA

Organizer: George E. Karniadakis Brown University, USA

Organizer: Mihai Anitescu Argonne National Laboratory, USA

Organizer: Omar Ghattas University of Texas at Austin, USA

#### 9:30-9:55 Scalable Algorithms for Bayesian Inverse Problems and Optimal Experimental Design with Applications to Large-scale Complex Systems

Alen Alexanderian, *Omar Ghattas*, Tobin Isaac, James R. Martin, Noemi Petra, and Georg Stadler, University of Texas at Austin, USA

### 10:00-10:25 Fast Kalman Filters for Seismic Imaging and CO2 Sequestration Monitoring

*Eric F. Darve*, Stanford University, USA; Sivaram Ambikasaran, Courant Institute of Mathematical Sciences, New York University, USA; Peter K. Kitanidis, Stanford University, USA; Judith Yue Li, Ruoxi Wang, and Hojat Ghorbanidehno, Stanford University, USA

#### 10:30-10:55 Numerical Upscaling Methods for Reservoir Model Reduction

Yahan Yang, ExxonMobil Upstream Research Company, USA; Xiaochen Wang, ExxonMobil, USA; Xiao-Hui Wu, ExxonMobil Upstream Research Company, USA

### 11:00-11:25 A Point-Process Approximation to Probability Measures of Spatially Varying Friction Coefficients

*Troy Butler*, University of Colorado, Denver, USA; Clint Dawson, University of Texas at Austin, USA; Don Estep, Colorado State University, USA; Lindley Graham, University of Texas at Austin, USA

### Thursday, April 3

## **MS87**

### Uncertainty Quantification via Dimension Reduction: Deterministic and Stochastic Approaches

### 9:30 AM-11:30 AM

### Room:Savannah Room - Lobby Level

Model reduction is crucial for quantifying uncertainties of largescale physical systems. It relies on the common assumption that many complex phenomena can be described by few selected features containing relevant information. Depending on the aim of the study, one may consider stochastic, deterministic or even mixed approaches, supervised or unsupervised tools. The goal of this minisymposium is to gather dimension reduction experts, who often mix various approaches in order to extract information they need for their problems, which can be e.g. inverse problems, non linear régression, sensitivity analysis. Assessment of reduced-order methods by a posteriori diagnostics are also proposed.

Organizer: Clémentine Prieur Universite Joseph Fourier and INRIA, France

### 9:30-9:55 Assesing Model Réduction for Sensitivity Analysis

*Clémentine Prieur*, Universite Joseph Fourier and INRIA, France; Alexandre Janon, Université Paris-Sud, France; Maelle Nodet, Grenoble University, France

### 10:00-10:25 Computational Reduction by Reduced Basis Methods for Inverse Problems Governed by PDEs

Andrea Manzoni, International School for Advanced Studies, Trieste, Italy

### 10:30-10:55 A Posteriori Error Estimates to Enable Effective Dimension Reduction in Stochastic Systems

*Tim Wildey*, Sandia National Laboratories, USA

### 11:00-11:25 Variable Selection for Quantifying Uncertainty Involving Functional Data

Simon Nanty, Commissariat à l'Energie Atomique, France; Céline Helbert, Ecole Centrale de Lyon, France; Amandine Marrel, CEA, France; Nadia Pérot, Commissariat à l'Energie Atomique, France; Clémentine Prieur, Universite Joseph Fourier and INRIA, France

# MS88

### Modern Topics in Optimum Experimental Design -Part I of II

9:30 AM-11:00 AM

Room: Plimsoll - Lobby Level

### For Part 2 see MS95

Methods for optimum experimental design (OED) are becoming more popular in industry and natural sciences by at least two reasons. First, increasing use of mathematical methods for modelbased simulation and optimization implies models validated by experiments. Secondly, OED offers the possibility to significantly reduce errors, experimental costs and time. Realization of methods in practice shows however, that in order to use the complete potential of nonlinear OED we have to deal with several new mathematical challenges which are addressed in this minisymposium: robust and online OED in order to reduce uncertainties, OED for PDE models, OED for new application areas.

Organizer: Stefan Körkel Heidelberg University, Germany

Organizer: Ekaterina Kostina Fachbereich Mathematik und Informatik, Philipps-Universität Marburg, Germany

Organizer: Mario S. Mommer Universität Heidelberg, Germany

### 9:30-9:55 Designing Experiments for Optimal Parameter Recovery in Biological Systems

Matthias Chung, Virginia Tech, USA

### 10:00-10:25 Robust Optimal Design of Experiments Based on a Higher Order Sensitivity Analysis

Max Nattermann, University of Marburg, Germany; Ekaterina Kostina, Fachbereich Mathematik und Informatik, Philipps-Universität Marburg, Germany

### 10:30-10:55 Online Model Validation

Stefan Körkel, Sebastian F. Walter, and Manuel Kudruss, Heidelberg University, Germany

### Lunch Break

11:30 AM-1:00 PM

Attendees on their own

Thursday, April 3

### IP8

### Recent Advances in Galerkin Methods for Parametric Uncertainty Propagation in Fluid Flow Simulations

1:00 PM-1:45 PM

Room:Ballroom A/B/C - 2nd Floor

Chair: Raul F. Tempone, King Abdullah University of Science & Technology (KAUST), Saudi Arabia

Application of stochastic spectral approximations for parametric uncertainty propagation in flow models governed by Navier-Stokes equations remains difficult because of computational complexity and possible non-smooth solutions (compressible flows). In this talk, I will first discuss recent developments in Proper Generalized Decompositions (PGD) and related algorithms. The application of PGD to the steady incompressible Navier-Stokes equations will illustrate the method and its computational complexity while highlighting limitations requiring further improvements. The second part of the talk will concern uncertain hyperbolic models and conservation laws with nonsmooth solutions, introducing a multiresolution framework with anisotropic adaptive strategy to control the local stochastic discretization in both space and time.

Olivier Le Maître LIMSI-CNRS, France

### Intermission

1:45 PM-2:00 PM

Thursday, April 3

## MT8

### Uncertainty Quantification Challenges in High-Performance Scientific Computing

2:00 PM-4:00 PM

Room:Ballroom A - 2nd Floor

Chair: Eric Phipps, Sandia National Laboratories, USA

Applying uncertainty quantification methodologies in high performance computing contexts presents numerous challenges such as expensive simulations, complex software frameworks, and the need to leverage advanced computer architecture capabilities. This minitutorial will explore techniques for improving performance of UQ methodologies in HPC applications by exposing new dimensions of fine-grained parallelism, improving memory access patterns, and extracting higher-order information, as well as approaches for applying these techniques in large, complex software code bases. This session is designed to complement MS96.

Eric Phipps, Sandia National Laboratories, USA

## **MS89**

### Numerical Methods for Uncertainty Quantification of Coupled Problems -Part IV of V

### 2:00 PM-4:00 PM

Room:Ballroom B - 2nd Floor

#### For Part 3 see MS79 For Part 5 see MS97

Accurate prediction of many engineering systems often requires simulations of tightly coupled and interacting phenomena with multiple physics or domains and at multiple scales. When uncertainties are present, the UO of such coupled systems is challenged by two difficulties. First, the presence of independent uncertainty sources within different physics/ scale models results in a combined high- dimensional stochastic space which may not be amenable to fast computation using standard approaches. Second, single physics/scale solvers are separate modules that may not have access to detailed information from one another. This minisymposium invites contributions that discuss the above challenges and provide novel solution techniques.

Organizer: Dongbin Xiu University of Utah, USA

Organizer: Alireza Doostan University of Colorado Boulder, USA

#### 2:00-2:25 Local Reduced Order Models for Stochastic Flows and Applications

Yalchin Efendiev, Texas A&M University, USA; Bangti Jin, University of California, Riverside, USA; Michael Presho and Xiaosi Tan, Texas A&M University, USA

#### 2:30-2:55 Uncertainty Quantification for Coupled Problems in Electronic Engineering

Roland Pulch, University of Greifswald, Germany; Sebastian Schöps, Technische Universitaet Darmstadt, Germany; Andreas Bartel, University of Wuppertal, Germany

### 3:00-3:25 The Stochastic Variational Multiscale Method: A Subgrid Model for Higher-order gPC with an In-built Error Indicator

Jayanth Jagalur-Mohan, Jason Li, and Onkar Sahni, Rensselaer Polytechnic Institute, USA; Alireza Doostan, University of Colorado Boulder, USA; *Assad Oberai*, Rensselaer Polytechnic Institute, USA

### 3:30-3:55 Uncertainty Quantification of Coupled Electrochemical Equations for the Simulation of Lithium-ion Batteries

Mohammad Hadigol and Alireza Doostan, University of Colorado Boulder, USA

## Thursday, April 3

# **MS90**

### Uncertainty Quantification and Models of Natural Hazards - Part I of II

2:00 PM-4:00 PM

Room:Ballroom D - 2nd Floor

### For Part 2 see MS98

Natural hazards such as volcanic eruptions, earthquakes and tsunamis are increasingly simulated using high performance computing due to their complexity (large domains at multiple scales, multi-physics). Uncertainty quantification is difficult for these models with uncertainties in parameterizations as well as source and boundary conditions. For warnings, time is critical and thus algorithms and design of computer experiments need to be tailored to the problem, with the aim to attach uncertainties to these warnings. For planning, the lack of long records makes UQ arduous. The minisymposium will examine various strategies for these challenges.

Organizer: Serge Guillas University College London, United Kingdom

Organizer: Abani K. Patra State University of New York, Buffalo, USA

Organizer: Elaine Spiller Marquette University, USA

### 2:00-2:25 Propagation of Uncertainties in Tsunami Modelling for the Pacific Northwest

Serge Guillas, Andria Sarri, Xiaoyu Liu, and Simon Day, University College London, United Kingdom; Frederic Dias, University College Dublin, Ireland

### 2:30-2:55 Can Small Islands Protect Nearby Coasts from Tsunamis?

Themistoklis Stefanakis, *Emile Contal*, and Nicolas Vayatis, ENS Cachan, France; Frederic Dias, University College Dublin, Ireland; Costas Synolakis, University of Southern California, USA

#### 3:00-3:25 Estimating the Maximum Earthquake Magnitude Based on Background Seismicity and Earthquake Clustering Characteristics

Jiancang Zhuang, Institute of Statistical Mathematics, Japan

# 3:30-3:55 Big Data Methods for Natural Hazard Analysis

Abani K. Patra, State University of New York, Buffalo, USA

2014 SIAM Conference on Uncertainty Quantification

Thursday, April 3

## MS91 Uncertainty Modeling for Complex Energy Systems

2:00 PM-4:00 PM

Room:Ballroom E - 2nd Floor

This minisymposium gathers techniques for uncertainty modeling and quantification motivated by power grid and building systems. We emphasize on decision-making as this motivates the development of new techniques. We cover areas such as Gaussian process modeling, Bayesian calibration of physical models, and scenario generation.

Organizer: Victor Zavala Argonne National Laboratory, USA

### 2:00-2:25 Gaussian Process Modeling with Incomplete Data: Applications to Building Systems

Victor Zavala, Argonne National Laboratory, USA

#### 2:30-2:55 Probabilistic Density Function Method for Stochastic Odes of Power Systems with Uncertain Power Input

Alexandre Tartakovsky, University of South Florida, USA; Peng Wang and Zhenyu Huang, Pacific Northwest National Laboratory, USA

### 3:00-3:25 Approximating Stochastic Process Models for Load and Wind Power in Stochastic Unit Commitment

Jean-Paul Watson, Sandia National Laboratories, USA; David Woodruff, University of California, Davis, USA; Sarah Ryan, Iowa State University, USA

#### 3:30-3:55 On the Role of Wind Correlation in Power Grid Stochastic Optimization Models

Cosmin G. Petra, Argonne National Laboratory, USA Thursday, April 3

## MS92

Theoretical and Numerical Analysis for Forward-Backward Stochastic Differential Equations and Stochastic Optimal Control -Part III of IV

2:00 PM-4:00 PM

Room:Ballroom F - 2nd Floor

### For Part 2 see MS82 For Part 4 see MS100 Forward-Backward SDEs (FBSDEs) have been widely studied in connection with partial differential equations, stochastic optimal control, nonlinear filtering and mathematical finance. The theoretical and numerical analyses of FBSDEs are more complicated than that of classical SDEs, so that there are many interesting and challenging open problems in this area. The minisymposium aims at exploring efforts related to theoretical and numerical analysis for FBSDEs including, but not limited to, BSDEs/FBSDEs theories, nonlinear expectations, FBDSDEs and nonlinear filtering, FBSDE-based stochastic optimal control, high-order numerical methods for FBSDEs, numerical solution for high-dimensional FBSDEs.

Organizer: Zhen Wu Shandong University, China

Organizer: Weidong Zhao Shandong University, China

Organizer: Guannan Zhang Oak Ridge National Laboratory, USA

### 2:00-2:25 Runge-Kutta Schemes for Backward Stochastic Differential Equations

Jean-François Chassagneux and Dan Crisan, Imperial College London, United Kingdom

### 2:30-2:55 A Stochastic Approach Via FBSDEs for Hyperbolic Conservation Laws

Yuanyuan Sui and Weidong Zhao, Shandong University, China; *Tao Zhou*, Chinese Academy of Sciences, China

### 3:00-3:25 Forward Backward Doubly Stochastic Differential Equations and Applications to The Optimal Filtering Problem

*Feng Bao* and Yanzhao Cao, Auburn University, USA

#### 3:30-3:55 Stochastic Control Systems Driven by Fractional Brownian Motions With Hurst Index H>1/2

Yuecai Han, Jilin University, China;Yaozhong Hu, University of Kansas, USA;Jian Song, University of Hong Kong,Hong Kong

continued in next column

## **MS93**

### Stochastic Models, UQ and Inversion of Large-scale High-dimensional Complex Systems - Part II of II

2:00 PM-3:30 PM

Room:Sloane Room - 2nd Floor

### For Part 1 see MS86

Our aim is to use accurate computational simulations to predict the behavior of complex systems. Many stochastic algorithms and techniques have been developed. The explosion in computational effort associated with the large number of random dimensions is often prohibitive, even for modern supercomputers. As such, advanced stochastic approximation techniques are necessary to minimize the complexity of mathematical models and make numerical solutions feasible. This minisymposium will explore recent advances in numerical algorithms and applications for uncertainty quantification, model reduction, and stochastic inversion in large-scale highdimensional complex systems.

Organizer: Guang Lin Pacific Northwest National Laboratory, USA

Organizer: George E. Karniadakis Brown University, USA

Organizer: Mihai Anitescu Argonne National Laboratory, USA

Organizer: Omar Ghattas University of Texas at Austin, USA

### 2:00-2:25 Robust Optimization with Chance Constraints in Noisy Regimes

*Florian Augustin* and Youssef M. Marzouk, Massachusetts Institute of Technology, USA

#### 2:30-2:55 Uncertainty Quantification of Dynamic Systems with Periodic Potentials

Peng Wang, Pacific Northwest National Laboratory, USA; *Xuan Zhang*, Daniel M. Tartakovsky, and Suiwen Wu, University of California, San Diego, USA; Alexander Tartakovsky, Pacific Northwest National Laboratory, USA

### 3:00-3:25 Uncertainty Quantification in DPD Simulations by Applying Compressive Sensing

Xiu Yang, Brown University, USA;Huan Lei, Pacific Northwest NationalLaboratory, USA; George E. Karniadakis,Brown University, USA

### Thursday, April 3

## MS94 Model Error and Model-form Uncertainty in CFD

2:00 PM-4:00 PM

Room:Savannah Room - Lobby Level

Computational Fluid Dynamics (CFD) is characterised by highly accurate representation of the majority of physics (e.g. conservation laws), combined with semi-empirical models for the remaining physics (usually for the small-scales). The error in simulation predictions due to these semi- empirical models is a matter of great importance for the trustworthiness of CFD. Recently Bayesian calibration has been used to optimise these models for specific flows. The work in this minisymposium goes further, attempting to (1) assess model-form uncertainty, and (2) devise stochastic estimates of model error. We cover two classes of modelling: turbulence closure modelling, and real-gas modelling for multi-phase and dense-gas flows.

Organizer: Richard Dwight Delft University of Technology, Netherlands

Organizer: Paola Cinnella ENSAM, ParisTech, France

#### 2:00-2:25 Quantification of Model-Form Uncertainty in Turbulence Closures

*Gianluca Iaccarino* and Michael Emory, Stanford University, USA; Catherine Gorle, University of Antwerp, Belgium

#### 2:30-2:55 Bayesian Model Average Estimates of Turbulence Closure Error

*Wouter Edeling*, TU Delft, Netherlands; Richard Dwight, Delft University of Technology, Netherlands; Paola Cinnella, ENSAM, ParisTech, France

#### 3:00-3:25 Evaluation of Real Gas Effects in Multiphase Flows Using Bayesian Inference and Uncertainty Quantification

*Remi Abgrall*, Pietro M. Congedo, and Maria-Giovanna Rodio, INRIA Bordeaux Sud-Ouest, France

### 3:30-3:55 Quantification of Model-Form Uncertainties in Thermodynamic Models for Dense Gas Flows

*Xavier Merle* and Paola Cinnella, ENSAM, ParisTech, France

## MS95 Modern Topics in Optimum

## Experimental Design -Part II of II

2:00 PM-3:30 PM

Room: Plimsoll - Lobby Level

### For Part 1 see MS88

Methods for optimum experimental design (OED) are becoming more popular in industry and natural sciences by at least two reasons. First, increasing use of mathematical methods for modelbased simulation and optimization implies models validated by experiments. Secondly, OED offers the possibility to significantly reduce errors, experimental costs and time. Realization of methods in practice shows however, that in order to use the complete potential of nonlinear OED we have to deal with several new mathematical challenges which are addressed in this minisymposium: robust and online OED in order to reduce uncertainties, OED for PDE models, OED for new application areas.

Organizer: Ekaterina Kostina Fachbereich Mathematik und Informatik, Philipps-Universität Marburg, Germany

Organizer: Stefan Körkel Heidelberg University, Germany

Organizer: Mario S. Mommer Universität Heidelberg, Germany

### 2:00-2:25 Computational Techniques for Experimental Design for III-Posed Problems

Jennifer Fohring and *Eldad Haber*, University of British Columbia, Canada

### 2:30-2:55 Bayesian Experimental Design for the Identification of Stochastic Reaction Dynamics

Heinz Koeppl, Christoph Zechner, and Michael Unger, ETH Zürich, Switzerland

#### 3:00-3:25 Optimum Experimental Design for Partial Differential Equations

Stefan Körkel, *Christoph Weiler*, and Andreas Schmidt, Heidelberg University, Germany Thursday, April 3

# CP16

### Biology and the Environment

2:00 PM-3:40 PM

Room: Verelst Room - 2nd Room

Chair: Bree Ettinger, Emory University, USA

### 2:00-2:15 First Passage Time for Uncertainty Quantifiaction of Numerical Environmental Models

Peter C. Chu, Naval Postgraduate School, USA

#### 2:20-2:35 Constructing the Energy Landscape for the Gene Regulatory Network with Intrinsic Noise *Tiejun Li*, Peking University, China

### 2:40-2:55 Validation and Uncertainty Quantification for Macroscale Soft Tissue Constitutive Models

*Kumar Vemaganti*, Sandeep Madireddy, and Bhargava Sista, University of Cincinnati, USA

#### 3:00-3:15 Multiple Patient Modeling over Bidimensional Riemannian Manifolds

Bree Ettinger, Emory University, USA; Simona Perotto and Laura M. Sangalli, Politecnico di Milano, Italy

#### 3:20-3:35 A Chaotic Model for Bird Flocking

Jorge Diaz-Castro, University of Puerto Rico, Puerto Rico

### Thursday, April 3

## CP17 Materials and Mechanics 2:00 PM-3:40 PM

Room: Percival Room - 2nd Floor

Chair: Gregory Bartram, Universal Technology Corporation, USA

### 2:00-2:15 Post-Optimality Analysis of Steel Production and Distribution

Abdallah A. Alshammari, King Fahd University of Petroleum and Minerals, Saudi Arabia

#### 2:20-2:35 Bayesian Network Identification of Thermal Buckling in Thin Beam Experiments

*Gregory Bartram*, Ricardo Perez, and Richard Wiebe, Universal Technology Corporation, USA; Benjamin P. Smarslok, Air Force Research Laboratory, USA

### 2:40-2:55 Uncertainty Quantification of Manufacturing Process Effects on Material Properties

*Guowei Cai* and Sankaran Mahadevan, Vanderbilt University, USA

#### 3:00-3:15 Bayesian Calibration of Thermal Buckling Models for Thin Panels

*Ricardo Perez*, Gregory Bartram, and Richard Wiebe, Universal Technology Corporation, USA; Benjamin P. Smarslok, Air Force Research Laboratory, USA

### 3:20-3:35 Identifying Sources of Model Uncertainty in Hypersonic Aerothermoelastic Predictions

Benjamin P. Smarslok, Air Force Research Laboratory, USA; Erin C. Decarlo, Vanderbilt University, USA; Ricardo Perez, Universal Technology Corporation, USA; Sankaran Mahadevan, Vanderbilt University, USA
Thursday, April 3

### CP18 Low-rank Approximations 2:00 PM-4:00 PM

Room:Vernon Room - 2nd Floor

Chair: Loïc Giraldi, Ecole Centrale de Nantes, France

### 2:00-2:15 Inverse Problems and Uncertainty Quantification: Low-Rank Matrix Inverse Approximations

Julianne Chung and Matthias Chung, Virginia Tech, USA

### 2:20-2:35 Non Intrusive Galerkin Method for Solving Stochastic Parametric Equations in Low-Rank Format

Loïc Giraldi, Ecole Centrale de Nantes, France; Alexander Litvinenko, King Abdullah University of Science & Technology (KAUST), Saudi Arabia; Dishi Liu, German Aerospace Center (DLR), Germany; Hermann G. Matthies, Technical University Braunschweig, Germany; Anthony Nouy, Ecole Centrale de Nantes, France

### 2:40-2:55 Dynamical Low Rank Approximation of Time Dependent Pdes with Random Data

*Eleonora Musharbash*, École Polytechnique Fédérale de Lausanne, Switzerland; Fabio Nobile, EPFL, France; Tao Zhou, Chinese Academy of Sciences, China

### 3:00-3:15 Low-Rank Solution of Unsteady Diffusion Equation with Stochastic Coefficients

Akwum Onwunta, Peter Benner, and Martin Stoll, Max Planck Institute, Magdeburg, Germany

### 3:20-3:35 Goal-Oriented Low-Rank Approximations for High Dimensional Stochastic Problems

*Olivier Zahm*, Marie Billaud-Friess, and Anthony Nouy, Ecole Centrale de Nantes, France

# 3:40-3:55 Variance Reduction Based $\ell_1$ -Minimization Methods for Sparse Approximation of Stochastic Partial Differential Equations

Ramakrishna Tipireddy, Guang Lin, and Zhijie Xu, Pacific Northwest National Laboratory, USA

### Coffee Break

4:00 PM-4:30 PM Room:Regency Foyer and

Promenade - 2nd Floor



### Thursday, April 3

### MS85 UQ That is Out of This World: UQ for Astronomy

4:30 PM-6:30 PM

Room: Vernon Room - 2nd Floor

A goal of this session is to bring interesting problems of astrophysics and cosmology to the attention of the UQ community. Much of the work done in astronomy has at least some connection to cosmological or astrophysical simulations, and the speakers of the this session will cover a variety of problems in astronomy. The proposed speakers include a theoretical cosmologist, a graduating astrophysics Ph.D. student, a computational astrophysicist, and a statistician. As one of the speakers pointed out, UQ needs to be emphasized in astrophysics, but it currently is not.

Organizer: Jessi Cisewski Carnegie Mellon University, USA

### 4:30-4:55 Numerical Methods with Quantifiable Errors for Astrophysical Simulation

Dinshaw Balsara, Notre Dame University, USA

5:00-5:25 Identification and Diagnostic of Transient Phenomena in Stellar Evolution

Tim Handy, Florida State University, USA

### 5:30-5:55 Approximate Sufficiency in Cosmological Estimation Problems Chad Schafer, Carnegie Mellon University, USA

### 6:00-6:25 Building the Cosmos: How Simulations Shed Light on the Dark Universe

Risa Wechsler, Stanford University, USA

### Thursday, April 3

### MS96 Uncertainty Quantification for Extreme-scale High Performance Computing

4:30 PM-6:30 PM

Room:Ballroom A - 2nd Floor

Applying uncertainty quantification methodologies in the context of high performance computing presents numerous challenges including expensive simulations, high dimensionality, simulations of complex multi-scale/multiphysics phenomena, and the necessity to deal with large simulation code software frameworks. Furthermore, the push to extreme-scaling computing requires simulations and uncertainty calculations implemented on emerging architectures to be able to exploit massive parallelism, limit communication and data motion, and be robust to hardware faults and failures. This minisymposium explores a variety of research areas focused on addressing these and other issues related to uncertainty quantification and high performance computing. This session is designed to complement MT8.

Organizer: Eric Phipps Sandia National Laboratories, USA

Organizer: Clayton G. Webster Oak Ridge National Laboratory, USA

### 4:30-4:55 Exploring Emerging Manycore Architectures for Uncertainty Quantification Through Embedded Stochastic Galerkin Methods

*Eric Phipps*, H. Carter Edwards, Jonathan J. Hu, and Jakob T. Ostien, Sandia National Laboratories, USA

### 5:00-5:25 Resilient Sparse Representation of Scientific Data for Uq on High Performance Computing

Richard Archibald and *Cory Hauck*, Oak Ridge National Laboratory, USA; Stanley J. Osher, University of California, Los Angeles, USA

continued on next page

Thursday, April 3

### **MS96**

Uncertainty Quantification for Extreme-scale High Performance Computing

4:30 PM-6:30 PM

continued

### 5:30-5:55 Probabilistic Approaches for Fault-Tolerance and Scalability in Extreme-Scale Computing

Bert J. Debusschere and Khachik Sargsyan, Sandia National Laboratories, USA; Francesco Rizzi, Duke University, USA; Cosmin Safta and Karla Morris, Sandia National Laboratories, USA; Omar M. Knio, Duke University, USA; Habib N. Najm, Sandia National Laboratories, USA

### 6:00-6:25 The Computational Complexity of Stochastic Galerkin and Collocation Methods for PDEs with Random Coefficients

Nick Dexter, University of Tennessee, USA; Miroslav Stoyanov and Clayton G. Webster, Oak Ridge National Laboratory, USA

### **MS97**

### Numerical Methods for Uncertainty Quantification of Coupled Problems -Part V of V

4:30 PM-6:30 PM

Room:Ballroom B - 2nd Floor

### For Part 4 see MS89

Accurate prediction of many engineering systems often requires simulations of tightly coupled and interacting phenomena with multiple physics or domains and at multiple scales. When uncertainties are present, the UQ of such coupled systems is challenged by two difficulties. First, the presence of independent uncertainty sources within different physics/scale models results in a combined high- dimensional stochastic space which may not be amenable to fast computation using standard approaches. Second, single physics/scale solvers are separate modules that may not have access to detailed information from one another. This minisymposium invites contributions that discuss the above challenges and provide novel solution techniques.

Organizer: Alireza Doostan University of Colorado Boulder, USA

Organizer: Dongbin Xiu University of Utah, USA

4:30-4:55 A Probabilistic Graphical Model Approach to Uncertainty Quantification for Multiscale Systems *Nicholas Zabaras*, Cornell University, USA

### 5:00-5:25 Stochastic Multiscale Analysis: a Benchmark Study in Materials Systems

Wei Chen and Wing Kam Liu, Northwestern University, USA

### 5:30-5:55 Random Discrete Least Square Polynomial Approximation for Pdes with Stochastic Data

*Fabio Nobile* and Giovanni Migliorati, EPFL, France; Raul F. Tempone, King Abdullah University of Science & Technology (KAUST), Saudi Arabia; Albert Cohen and Abdellah Chkifa, Université Pierre et Marie Curie, France

### 6:00-6:25 A Probabilistic Method for Efficient Behavior Classification

*Gregery Buzzard*, Vu Dinh, and Ann E. Rundell, Purdue University, USA

### Thursday, April 3

### **MS98**

### Uncertainty Quantification and Models of Natural Hazards - Part II of II

4:30 PM-6:30 PM

Room:Ballroom D - 2nd Floor

### For Part 1 see MS90

Natural hazards such as volcanic eruptions, earthquakes and tsunamis are increasingly simulated using high performance computing due to their complexity (large domains at multiple scales, multi-physics). Uncertainty quantification is difficult for these models with uncertainties in parameterizations as well as source and boundary conditions. For warnings, time is critical and thus algorithms and design of computer experiments need to be tailored to the problem, with the aim to attach uncertainties to these warnings. For planning, the lack of long records makes UQ arduous. The minisymposium will examine various strategies for these challenges.

Organizer: Serge Guillas University College London, United Kingdom

Organizer: Abani K. Patra State University of New York, Buffalo, USA

Organizer: Elaine Spiller Marquette University, USA

### 4:30-4:55 Where Are You Gonna Go When the Volcano Blows?

*E. Bruce Pitman*, State University of New York, Buffalo, USA; James Berger and Robert L. Wolpert, Duke University, USA; Abani K. Patra, State University of New York, Buffalo, USA; Elaine Spiller, Marquette University, USA; Susie Bayarri, University of Valencia, Spain; Eliza Calder, University of Edinburgh, United Kingdom

### 5:00-5:25 Improved and Fast Gasp Emulation Strategies

Susie Bayarri, University of Valencia, Spain; James Berger, Duke University, USA; Eliza Calder, University of Edinburgh, United Kingdom; Abani K. Patra and E. Bruce Pitman, State University of New York, Buffalo, USA; Elaine Spiller, Marquette University, USA; Robert L. Wolpert, Duke University, USA

### 5:30-5:55 Combinbing Multiple Sources of Uncertainty in Geophysical Hazard Mapping

Elaine Spiller, Marquette University, USA

### 6:00-6:25 Parallel Thinning

Robert L. Wolpert and Mary E. Broadbent, Duke University, USA

### Thursday, April 3

## MS99 HPC Meets UQ - Part II of II

4:30 PM-6:30 PM

### Room:Ballroom E - 2nd Floor

### For Part 1 see MS81

Uncertainty quantification increases the insight that can be gained through simulations in CSE at the price of significantly increased complexity. Besides the need for sophisticated mathematical approaches, performing UQ typically multiplies the computational costs by several orders of magnitude compared to the single deterministic simulations. Thus, high-performance computing aspects are ubiquitous in UQ across various disciplines and applications. The combination of these two fields is highly relevant and challenging, in particular with respect to the paradigm shifts in HPC in the era of massively parallel computing. This minisymposium is organised in collaboration with the German Priority Programme SPPEXA "Software for Exascale Computing" and addresses aspects of HPC in UQ.

Organizer: Tobias Neckel TU München, Germany

Organizer: George Biros University of Texas at Austin, USA

Organizer: Dirk Pflüger Universität Stuttgart, Germany

### 4:30-4:55 Dakota Infrastructure and Algorithms Enabling Advanced UQ

Brian M. Adams, *Patricia D. Hough*, and Laura Swiler, Sandia National Laboratories, USA

### 5:00-5:25 Advances and Challenges of Uncertainty Quantification with Application to Climate Prediction

Richard I. Klein, Lawrence Livermore National Laboratory, USA

### 5:30-5:55 Scalable Gaussian Process Analysis

*Mihai Anitescu* and Jie Chen, Argonne National Laboratory, USA; Michael Stein, University of Chicago, USA

### 6:00-6:25 Statistical Inversion for Basal Parameters for the Antarctic Ice Sheet

*Tobin Isaac*, Noemi Petra, Georg Stadler, and Omar Ghattas, University of Texas at Austin, USA

### Thursday, April 3

### MS100

Theoretical and Numerical Analysis for Forward-Backward Stochastic Differential Equations and Stochastic Optimal Control -Part IV of IV

4:30 PM-6:30 PM

Room:Ballroom F - 2nd Floor

### For Part 3 see MS92

Forward-Backward SDEs (FBSDEs) have been widely studied in connection with partial differential equations, stochastic optimal control, nonlinear filtering and mathematical finance. The theoretical and numerical analyses of FBSDEs are more complicated than that of classical SDEs, so that there are many interesting and challenging open problems in this area. The minisymposium aims at exploring efforts related to theoretical and numerical analysis for FBSDEs including, but not limited to, BSDEs/ FBSDEs theories, nonlinear expectations, FBDSDEs and nonlinear filtering, FBSDE-based stochastic optimal control, high-order numerical methods for FBSDEs, numerical solution for highdimensional FBSDEs.

Organizer: Zhen Wu Shandong University, China

Organizer: Weidong Zhao Shandong University, China

Organizer: Guannan Zhang Oak Ridge National Laboratory, USA

### 4:30-4:55 Value in Mixed Strategies for Zero-Sum Stochastic Differential Games Without Isaacs Condition

Juan Li, Shandong University, China; Rainer Buckdahn and Marc Quincampoix, Universite de Brest, France

### 5:00-5:25 Robust Utility Maximisation Via Second Order BSDEs

Anis Matoussi, University of Maine, USA; Dylan Possamaï, CEREMADE Universite Paris 9 Dauphine, France; *Chao Zhou*, National University of Singapore, Singapore

continued on next page

Thursday, April 3

### MS100

Theoretical and Numerical Analysis for Forward-Backward Stochastic Differential Equations and Stochastic Optimal Control -Part IV of IV

4:30 PM-6:30 PM

continued

5:30-5:55 Stochastic Control Representations for Penalized Backward Stochastic Differential Equations

Gechun Liang, University of Oxford, United Kingdom

### 6:00-6:25 Split-step Milstein Methods for Multi-channel Stiff Stochastic Differential Systems

Viktor Reshniak and Abdul Khaliq, Middle Tennessee State University, USA; David A. Voss, Western Illinois University, USA

# UQ14 Abstracts



Abstracts are printed as submitted by the authors.

### IP1

### Quantifying Uncertainty in Multiscale Heterogenous Solid Earth Crustal Deformation Data to Improve Understanding of Earthquake Processes

Earthquakes can cause tremendous loss of life and property yet predicting the behavior of earthquake fault systems is exceptionally difficult. The Earths crust is complex and earthquakes generate at depth, which is problematic for understanding earthquake fault behavior. Geodetic imaging observations of crustal deformation from Global Positioning System (GPS) and Interferometric Synthetic Aperture Radar (InSAR) measurements make it possible to characterize interseismic and aseismic motions, complementing seismic and geologic observations. Earthquake processes and the associated data are multiscale in the spatial and temporal domains making it particularly difficult to quantify uncertainty. Fusing the observations results in better understanding of earthquake processes and characterization of the uncertainties of each data type.

#### Andrea Donnellan

Jet Propulsion Laboratory & Univ of Southern California Deputy Manager, Exploration Systems Autonomy donnellan@jpl.nasa.gov

### IP2

#### Uncertainty Quantification in Nonparametric Regression and Ill-posed Inverse Problems

The problem of recovering useful functional information from discrete heterogenous, scattered, noisy, incomplete observational information and prior assumptions concerning the nature of the desired function is ubiquitous in many fields, including numerical weather prediction and biomedical risk factor modeling. In parallel we have the problem of quantifying the uncertainty in the functional estimates. We will cast this problem in an applicable, but somewhat abstract form as an optimization problem in a Reproducing kernel Hilbert space and discuss the role of cross validation in the trade offs in combining observational data and prior assumptions in functional estimation as well as in modeling uncertainty in the estimates.

<u>Grace Wahba</u> Department of Statistics University of Wisconsin-Madison wahba@stat.wisc.edu

### IP3

#### Uncertainty Quantification in Bayesian Inversion

Many problems in the physical sciences require the determination of an unknown field from a finite set of indirect measurements. Examples include oceanography, oil recovery, water resource management and weather forecasting. The Bayesian approach to these problems provides a natural way to provide estimates of the unknown field, together with a quantification of the uncertainty associated with the estimate. In this talk I will describe an emerging mathematical framework for these problems, explaining the resulting well-posedness and stability theory, and showing how it leads to novel computational algorithms. This session was designed to complement MS27.

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

### IP4

### Evidence-based Treatment of Computer Experiments

Using a complex computer model for optimization, sensitivity analysis, etc. typically requires a surrogate (approximation) to enable many (fast) predictions. Building a surrogate is done via a set of runs at designated inputs that is, a computer experiment. Choices must be made to design the experiment and build the surrogate: Design – How many runs? At what inputs? Methods for Surrogate Building – Polynomial chaos (PC)? Gaussian process Bayesian methods (GP)? Specifics of Methods – Which PC? Which GP? Faced with a myriad of competing answers what's a modeler to do? Does it matter? The talk, based on work with John Jakeman, Jason Loeppky and William Welch, will describe an evidence-based approach to compare and evaluate competing methods leading to recommendations and findings, some at variance with common beliefs.

#### Jerome Sacks

National Institute of Statistical Sciences sacks@niss.org

### $\mathbf{IP5}$

### Gaussian Process Emulation of Computer Models with Massive Output

Often computer models yield massive output, such as temperature over a large grid of space and time. Emulation (i.e., developing a fast approximation) of the computer model can then be particularly challenging. Approaches that have been considered include utilization of multivariate emulators, modeling of the output (e.g., through some basis representation, including PCA), and construction of parallel emulators at each grid point. These approaches will be reviewed, with the startling computational simplicity with which the last approach can be implemented being highlighted. Illustrations with computer models of pyroclastic flow and wind fields will be given.

James Berger, Mengyang Gu Duke University berger@stat.duke.edu, mg211@stat.duke.edu

### IP6

#### The Theory Behind Reduced Basis Methods

Reduced basis methods are a popular numerical tool for solving parametric and stochastic partial differential equations. We will discuss the theory behind such methods in the case of elliptic parametric equations. The main question we will answer is when can we know a priori that these methods will perform better than simply calling on a standard Finite Element Solver or Adaptive Finite Element Solver. We shall see that this is related to the smoothness of the manifold of solutions and in particular to the Kolmogorov width of this manifold. We will also discuss when a particular implementation of reduced basis methods known as greedy algorithms will guarantee optimal performance.

 $\frac{\text{Ronald DeVore}}{\text{Texas A&M University}}$ 

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### $\mathbf{IP7}$

#### Uncertainties Without the Rev. Thomas Bayes

Inverse problems in geophysics always fail to have unique solutions because of incompleteness of the measurements. None-the-less, it is often possible to obtain valuable insights by formulating a suitable optimization problem and thereby bounding some useful property, such as the average value in a region. Examples will be given from planetary science, bore-hole well logging of NRM data, and electromagnetic sounding.

<u>Robert Parker</u> University of California San Diego RLPARKER@UCSD.EDU

### IP8

### Recent Advances in Galerkin Methods for Parametric Uncertainty Propagation in Fluid Flow Simulations

Application of stochastic spectral approximations for parametric uncertainty propagation in flow models governed by Navier-Stokes equations remains difficult because of computational complexity and possible non-smooth solutions (compressible flows). In this talk, I will first discuss recent developments in Proper Generalized Decompositions (PGD) and related algorithms. The application of PGD to the steady incompressible Navier-Stokes equations will illustrate the method and its computational complexity while highlighting limitations requiring further improvements. The second part of the talk will concern uncertain hyperbolic models and conservation laws with non-smooth solutions, introducing a multi-resolution framework with anisotropic adaptive strategy to control the local stochastic discretization in both space and time.

### <u>Olivier Le Matre</u>

Laboratoire d'Informatique pour la Mécanique et les Sciences LIMSI-CNRS & Duke University olm@limsi.fr

### $\mathbf{CP1}$

### Model Fidelity Effect on Calibration of System Parameters

This presentation discusses the uncertainty in model parameter estimation due to choices of fidelity. It presents a strategy to balance accuracy and effort through an optimum combination of low and high fidelity simulations and correction of the low-fidelity model. The application example considers damping estimation of a curved panel located near a hypersonic vehicle engine, and subjected to structural, acoustic and thermal loading. The models range from quasi-static to reduced-order to full transient analysis.

<u>Ghina N. Absi</u>, Sankaran Mahadevan Vanderbilt University ghina.nakad@vanderbilt.edu, sankaran.mahadevan@vanderbilt.edu

#### CP1

Parameter Identification Via Sensitivity and Opti-

#### mization

We study a model of a biochemical cascade, triggered by photons in retinal photoreceptors, which constitutes the first stage of vision. The cascade, with multi-stage shutoff of activated rhodopsin, is described by 70 reactions involving 16 primary parameters. A sensitivity analysis suggests that 4 of the parameters affect the response the most. We present an optimization approach to find parameters that result in desired peak and timing of response matching experimental data.

Vasilios Alexiades

Department of Mathematics University of Tennessee, Knoxville alexiades@utk.edu

### $\mathbf{CP1}$

### New Index Theory Based Algorithm for the Gravity Gradiometer Inverse Source Problem

We present a new algorithm designed to improve the gravity gradiometer inverse solution. Our gradiometer observable is a symmetric, trace-free, 2-tensor. The algorithm leverages Index Theory, which relates changes in index values computed on a closed curve containing a line field generated by the positive eigenvector of the gradiometer tensor to the closeness of fit of the proposed inverse solution to the mass and center of mass of the unknown anomaly.

<u>Robert C. Anderson</u>, Jonathan Fitton National Geospatial-Intelligence Agency robert.c.anderson@nga.mil, jonathan.w.fitton@nga.mil

#### CP1

# Entropy-Bayesian Inversion of Hydrological Parameters in the Community Land Model Using Heat Flux and Runoff Data

We present results of parameter calibration at several flux tower sites and MOPEX basins using an Entropy-Bayesian inversion approach integrated with the Community Land Model (CLM). The approach updates probability distributions of the unknown parameters at each stage, when a new and supplementary ensemble set of samples are generated adaptively from the updated intermediate priors. The corresponding CLM numerical evaluations can be conducted efficiently in a task-parallel manner.

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

### $\mathbf{CP1}$

#### Parameter Identification in a Bayesian Setting

Our lack of knowledge or the uncertainty of the actual value of the parameter can be described in a Bayesian way through a probabilistic model. Such a description has two constituents, the measurable function and the measure. One group of methods is identified as updating the measure, the other group changes the measurable function. We connect both groups with the methods of functional approximation of stochastic problems, and hence introduce a new procedure which works completely deterministically.

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Hermann Matthies Technische Universität Braunschweig wire@tu-braunschweig.de

### CP1

### Parameter Estimation and Uncertainty Quantification of Coupled Reservoir and Geomechanical Modeling at a Co2 Injection Site

Parameter estimation and uncertainty quantification of coupled reservoir and geomechanical simulations during CO2 sequestration requires a computationally efficient framework. We estimate key hydrogeologic features to govern the geomechanical response at a CO2 injection project at In Salah, Algeria. Observed data include surface uplifts and pore-pressure increase in the CO2 injection zone. Null-space Monte Carlo and polynomial chaos expansion methods are applied for enhancing our understanding of coupled multi-physics associated with the CO2 injection.

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Steven Bryant

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### $\mathbf{CP2}$

### Numerical Integration Error-Based Innovation in Ensemble Kalman Filters

Ensemble Kalman filtering techniques have been developed to perform state estimation for large, turbulent nonlinear dynamical systems. We propose a stochastic interpretation of the discretization error in numerical integrators to extend the technique to deterministic, large-scale nonlinear evolution models, with innovation variance based on classical error estimates. The effectiveness of the resulting algorithm is demonstrated on the Lorenz-63 model and an application to skeletal muscle metabolism.

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Daniela Calvetti Case Western Reserve Univ Department of Mathematics dxc57@case.edu

Erkki Somersalo Case Western Reserve University ejs49@case.edu

### $\mathbf{CP2}$

### Quantile Estimation for Numerical Solution of Differential Equations with Random Data

High or low quantiles give information about the tail of a distribution and hence about rare or extreme outcomes. In this talk, we present a Monte Carlo-based algorithm for estimating a p-quantile error bound of a distribution generated by a functional of the solution to a differential equation with uncertain data. Functional error estimates determine at what accuracy realizations should be solved to achieve an accurate bound at reduced computational cost.

<u>Fredrik Hellman</u> Department of Information Technology Uppsala University fredrik.hellman@it.uu.se

Daniel Elfverson Uppsala University (Sweden), Div. Scientific Computing Dept. Information Technology daniel.elfverson@it.uu.se

Donald Estep Department of Statistics Colorado State University estep@stat.colostate.edu

Axel Målqvist Department of Information Technology Uppsala University axel.malqvist@it.uu.se

### $\mathbf{CP2}$

### Convergence of Square Root Ensemble Kalman Filters in the Large Ensemble Limit

Unbiased square root ensemble filters use deterministic algorithms to produce an analysis (posterior) ensemble with prescribed mean and covariance consistent with the Kalman update. We show that at every time index, as the number of ensemble members increases to infinity, the mean and covariance of an unbiased ensemble square root filter converge to those of the Kalman filter. The convergence is in  $L^p$  and the convergence rate does not depend on the model dimension.

Evan Kwiatkowski, Jan Mandel University of Colorado at Denver evan.kwiatkowski@ucdenver.edu, jan.mandel@ucdenver.edu

### $\mathbf{CP2}$

### 4DVAR by Ensemble Kalman Smoother

The ensemble Kalman smoother (EnKS) is used as a linear least squares solver in the Gauss-Newton method for the large nonlinear least squares in incremental 4DVAR. The ensemble approach is naturally parallel and no tangent or adjoint operators are needed. Adding a regularization term results in replacing the Gauss-Newton method, which may diverge, by convergent Levenberg-Marquardt method. The regularization is implemented as an additional observation in the EnKS.

#### Jan Mandel

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### $\mathbf{CP2}$

### Reduced Variance by Robust Design of Boundary Conditions for a Hyperbolic System of Equations

The connection between the boundary conditions and the variance of the solution to a stochastic partial differential equation (PDE) are investigated. In particular a hyperbolical system of PDEs with stochastic initial and boundary data are considered. The problem is shown to be well-posed for a class of boundary conditions through the energy method. Stability is shown by using summation-by-part operators with weak boundary procedures. By using the energy-method, the relative variance of the solutions for different boundary conditions are analyzed. It is concluded that some types of boundary conditions yields a lower variance than others. This is verified by numerical computations.

#### Jan Nordstrom

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Markus Wahlsten Department of Mathematics Linköping University SE 581 83 Linköping, Sweden markus.wahlsten@liu.se

#### $\mathbf{CP2}$

### Uncertainty Quantification of One Dimensional Steady State Second Order Pdes with Random Coefficients: An Analytical Study

We will present an analytical study to estimate the output uncertainty for a general class of second order steady state PDEs with random coefficients with given covariance function. The mean and the variance of the output at any given location can be explicitly written in terms of the mean, the variance, and the correlation length of the random coefficients. The dependence of the output variance on the correlation length can be compared with numerical results.

### Zhijie Xu

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Ramakrishna Tipireddy University of Southern California ramakrishna.tipireddy@pnnl.gov

Guang Lin Pacific Northwest National Laboratory guang.lin@pnnl.gov

### CP3

### Climate Change and Public Health, Accounting for Uncertainty Between Air Quality and Asthma

Climate change projections based on high resolution regional climate and air quality models are used quantify the subsequent impacts on asthma-related health effects. Two key sources of uncertainty are in the climate projections themselves and in the relationship between air quality and asthma. Bayesian hierarchical models provide a statistical relationship between asthma and future air pollution levels, and naturally allow the propagation of uncertainty through to public health outcomes.

#### Stacey Alexeeff

National Center for Atmospheric Research salexeef@ucar.edu

### CP3

### Two Approaches to Calibration in Metrology

Inferring mathematical relationships with quantified uncertainty from measurement data is common to computational science and metrology. Sufficient knowledge of measurement process noise enables Bayesian inference. Otherwise, an alternative approach is required, here termed *compartmentalized inference*, because collection of uncertain data and model inference occur independently. Bayesian parameterized model inference is compared to a Bayesian-compatible compartmentalized approach for ISO-GUM compliant calibration problems in renewable energy metrology. In either approach, model evidence can help reduce model discrepancy.

Mark Campanelli

National Institute of Standards and Technology mark.campanelli@nrel.gov

### CP3

### Uncertainty Qualification in Hurricane Risk Assessment

Each year hurricanes cause extensive economic loss and social disruption all around the world. Annual hurricane economic loss in the United States has been \$10 billion in recent years. Various hurricane wind field models have been proposed, and hurricane loss has been estimated based on these models. This paper examines uncertainty in hurricane risk assessment. In this paper, we describe the spatial correlation structure of hurricane wind fields and introduce the calculation of the spatial correlation using software R. The data from Hurricane Ivan (2004) is used to quantify the spatial correlations in wind field. Our analysis qualitatively determines the spatial correlation in the hurricane wind fields.

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### $\mathbf{CP3}$

### Multi-Model Ensemble Assimilation for Enhance Model Prediction: Specification of Ionosphere-Thermosphere Environment

The simulation of complex physical phenomena is commonplace in many areas of science. A concern is that model errors and bias, resulting from uncertain parameters and unaccounted physical processes, have a significant influence on model forecast accuracy. In this talk we present a multi-model ensemble system coupled with an assimilation algorithm to improve the forecast of the ionospherethermosphere environment. The main advantage of our approach is that combining a number of models can help mitigate model errors suffered by any one model. A number of numerical experiments are presented which compare the forecast performance of assimilation with single-model and multi-model techniques.

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### CP3

### Quantifying Initial Conditions Uncertainty in Gulf of Mexico Circulation Forecasts Using a Non-Intrusive Polynomial Chaos Method

Generalized polynomial chaos are applied to study the uncertainty in initial conditions in the Gulf of Mexico using HyCOM. A 14-day simulation provides the EOFs which are the characteristic modes of variability in the system. The leading modes are scaled stochastically and added to the initial conditions of a control run. The ensuing uncertainty is propagated through the system using a nonintrusive formalism. The results are presented along with potential applications to oil fate modeling.

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### CP3

### Sensitivity Analysis of Coupled Flow and Geomechanical Effects on Predictining the Surface Uplift at InSalah

The InSalah project in Algeria is a pioneering industrialscale demonstration of  $CO_2$  capture and storage. Over a five-year period, 3 million tones  $CO_2$  has been injected into sandstone reservoir located at about 1800-1900 m below the surface ground. In this study, Sierra Toolkits- an engineering mechanics simulation code developed at Sandia National Laboratories- is adopted to simulate this coupled multi-physics problem. The sensitivity analysis is performed to investigate the potential causes of the uplift.

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### $\mathbf{CP4}$

### Uncertainty Quantification for Robust Optimization: Information Theory and Extended Relational Algebra of Polytopes

Our hierarchical representation of uncertainty using constraints on aggregates, sums, differences, etc. of uncertain parameters enables the use of incremental LP techniques and also allows simple quantification of amount of information driving the optimization. Our robust uncertainty quantification is computationally simpler than probabilistic alternatives and incorporates the worst case over an infinite scenario ensemble. Using an extended relational algebra of polytopes, we can also qualitatively compare and visualize the relationships among alternative constraint sets.

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### $\mathbf{CP4}$

### A Multigrid Method for Optimal Control Problems Constrained by Elliptic Equations with Stochastic Diffusion Coefficients

We present a multigrid algorithm for an optimal control problem constrained by a linear elliptic equation with stochastic diffusion coefficient. Assuming a finite Karhuenen-Loéve expansion for the diffusion coefficient, we discretize the optimization problem by first discretizing the elliptic equation using a stochastic Galerkin formulation. We show how the potentially large-scale KKT system of the resulting discrete optimization problem can be solved efficiently using multigrid methods inherited from the associated deterministic elliptic-constrained problem.

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### CP4

### Uqlab: An Advanced Software Framework for Uncertainty Quantification

The UQLab project is a MATLAB-based software framework designed to enable industrial and academic users to use and develop advanced uncertainty quantification algorithms. Its design is flexible and easy to extend by scientists without extensive IT background, while providing an interface to common High Performance Computing facilities. So far it includes modules for reliability and surrogate modeling (e.g., advanced polynomial chaos expansion and Kriging algorithms). This contribution gives an overview of the current platform capabilities.

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### $\mathbf{CP4}$

### Multigrid Preconditioners for Stochastic Optimal Control Problems with Elliptic Spde Constraints

We consider an optimal control problem constrained by an elliptic SPDE, with a stochastic cost functional of tracking type. We use a sparse grid stochastic collocation approach to discretize in the probability space and finite elements to discretize in the physical space. To accelerate the solution process, we propose a deterministic multigrid preconditioner for the stochastic reduced KKT system, similar to the preconditioners introduced by Draganescu and Dupont for the deterministic PDE constrained problem.

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### $\mathbf{CP4}$

### Hierarchical Preconditioners in the Context of Stochastic Galerkin Finite Elements

Stochastic Galerkin finite element discretizations lead to very large systems of linear equations that are thus solved iteratively. We propose a family of preconditioners that take advantage of (the recursion in) the hierarchy of the global system matrices. Neither the global matrix nor the preconditioner need to be formed explicitly, and ingredients include only the stiffness matrices from the polynomial chaos expansion and a preconditioner for the mean-value problem. Besides utilizing the preconditioners with Krylov subspace iterative methods, we also apply them in the context of iterative solution of eigenvalue problems, e.g., by the inverse subspace iterations. The performance is illustrated by numerical experiments.

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### $\mathbf{CP4}$

### A New Uncertainty-Bearing Floating-Point Arithmetic

A new deterministic floating-point arithmetic called precision arithmetic is developed to track precision for arithmetic calculations. It uses a novel rounding scheme to avoid the excessive rounding error propagation of conventional floating-point arithmetic. Unlike interval arithmetic, its uncertainty tracking is based on statistics and the central limit theorem, with a much tighter bounding range. Its stable rounding error distribution is approximated by a truncated Gaussian distribution. Generic standards and systematic methods for comparing uncertaintybearing arithmetics are discussed. The precision arithmetic is found to be superior to interval arithmetic in both uncertainty-tracking and uncertainty-bounding for normal usages. Particularly, the precision arithmetic satisfies two characteristics: 1) expression independency; and 2) recovery of input uncertainty after a round-trip transformation. The arithmetic code is published at http://precisionarithm.sourceforge.net, while the full article is published at http://arxiv.org/abs/cs/0606103.

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### $\mathbf{CP5}$

# $L_2$ -Boosting on Generalized Hoeffding Decomposition for Dependent Variables - Application to Sensitivity Analysis

We are interested in the Hierarchically Orthogonal Functional Decomposition of any function to estimate Sobol indexes for uncertainty quantification. To estimate the HOFD components, we propose to construct recursively a basis that satisfies the constraints and is close to the theoretical one. Then, the unknown coefficients of the decomposition are deduced by  $L_2$ -boosting algorithm. When the number of observations tends to infinity, this algorithm recovers the true function with high probability.

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### CP5

### New Sensitivity Analysis Subordinated to a Contrast

In a model of the form  $Y = h(X_1, \ldots, X_d)$  where the goal is to estimate a parameter of the probability distribution of Y, Sobol indices are usually used to quantify the importance of each variable  $X_i$ . Nevertheless, we show in this work, that those indices are not always well adapted depending on what we want to estimate. Hence the aim of this work is to show how to define *goal oriented sensitivity indices* that are well suited for quantifying the importance of each variable  $X_i$  with respect to the quantity of interest. In this framework, we will show that Sobol indices are sensitivity indices associated to a particular characteristic of the distribution Y, the mean!!

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#### $\mathbf{CP5}$

### Morris Screening Combined with Gaussian Process-Based Joint Metamodels for the Sensitivity Analysis of Simulation Codes

We combine a screening method with a joint metamodeling to perform the sensitivity analysis of computer codes. First, a Morris screening is performed. From this, the inputs are split into two groups: the influential (Gp1) and the negligible ones (Gp2). Then, a Gaussian processbased joint metamodel is used to fit the mean and the heteroscedastic output variance against the Gp1 variables. Sobol sensitivity indices are estimated to confirm the relevance of Morris graph interpretation.

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#### $\mathbf{CP5}$

### Experience with Selected Methods for Sensitivity Analysis of a Computational Model with Quasi-Discrete Behavior

Different methods of sensitivity analysis were applied to a performance assessment model for a final repository for low and intermediate level radioactive waste in rock salt. With respect to specific input parameters, this model shows a quasi-discrete behavior, which seems to be the reason for the major differences in parameter ranking that were obtained, depending on the type of methods.

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### CP5

#### Efficiency of Monte Carlo Parameter Sensitivity Estimators for Chemical Kinetics

It has been observed that the pathwise derivative (PD) approach has lower variance than the Girsanov transformation (GT) method in the estimation of parametric sensitivities for stochastic dynamical systems. We give a justification for this observation when system size N is modestly large for density dependent systems. In the context of chemical kinetics we show that the relative error of the

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### CP6

### Uncertainty Quantification in Mesoscopic Modeling and Simulation

We propose a method to quantify the parameter induced uncertainties in a mesoscopic simulation by employing the compressive sensing method to compute the coefficients of the generalized polynomial chaos (gPC) expansion. We utilize the constructed gPC expansion to investigate the intrinsic relationship between the different model parameters and identify the degeneracy of the parameter space ; hence it helps us to remove the modeling redundancies of the mesoscopic system.

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### CP6

### Resource Allocation for Uncertainty Quantification and Reduction

Computational models are required to predict behavior in regimes of interest where test data is unavailable, so they are calibrated and validated at lower levels where tests are feasible. They are then used in predictive simulations to propagate uncertainty (both aleatory and epistemic) to the output of interest. This research uses Bayesian networkbased calibration/validation and surrogate-based optimization for model and test selection to perform uncertainty quantification subject to budget constraints.

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### $\mathbf{CP6}$

### Quantification of Aleatory and Epistemic Uncertainties in Reliability Assessment

A probabilistic framework to include both aleatory and epistemic uncertainties in reliability assessment is proposed, and demonstrated for an aircraft wing. Epistemic uncertainty due to data and model sources is included through auxiliary variables, resulting in an efficient singleloop computational approach. Uncertainties in distribution types, distribution parameters, and correlations, due to sparse or imprecise data regarding input variables, are included. Model errors (numerical solution errors and model form errors) are quantified through Gaussian process models.

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### CP6

### Stochastic Polynomial Interpolation for Uncertainty Quantification with Computer Experiments

Multivariate polynomial metamodels are widely used for uncertainty quantification due to the development of stochastic collocation. However, these metamodels only provide point predictions. There is no known method that can quantify interpolation error probabilistically and design interpolation points using available data to reduce the error. We shall introduce the stochastic interpolating polynomial model, which overcomes these problems. A Bayesian approach that quantifies interpolation uncertainty through the posterior distribution of the output is taken.

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### $\mathbf{CP6}$

### Algebraic Quadrature for Uncertainty Quantification

An algebraic quadrature method based on the theory of zero dimensional algebraic varieties is proposed. The method generates quadrature weights for arbitrary random input designs to create a numerical quadrature with a known polynomial order of accuracy and is shown to be a general method for quadrature weight generation for any classical Gauss and Smolyak quadratures. The accuracy of the algebraic quadrature is compared to these classical quadratures in the context polynomial chaos expansion and probabilistic collocation.

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### $\mathbf{CP6}$

### Analysis for the Least Square Approach with Applications for Uncertainty Quantification

In this talk, we discuss the least square approach on high dimensional polynomial spaces. A possible application for such method is uncertainty quantifications. Unlike the traditional random sampling method, we consder in this work the use of specially designed deterministic points. Stability and convergence results will be shown. Numerical tests show that the deterministic points admit similar performance with that of the random points.

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### CP7

### Multilevel Monte Carlo Methods for Rare Event Probabilities and Quantiles

Differential equations with uncertainty in the data arise in many different fields in computational sciences. Often one is not interested in the solution of a differential equations directly but rather a particular functional of the solution, a quantity of interest. In this work we focus on estimating rare event probabilities and quantiles. We combine recent results on quantile estimation with Multilevel Monte Carlo methods with promising results.

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### CP7

### Optimization of Mesh Hierarchies for Multilevel Monte Carlo

We consider the Multilevel Monte Carlo (MLMC) method in applications involving differential equations with random data where the underlying approximation method of individual samples is based on uniform spatial discretizations of arbitrary approximation order and cost. We perform a general optimization of the parameters defining the MLMC hierarchy in such cases. The resulting hierarchies are different from typical MLMC hierarchies in that they do not have a fixed ratio between successive mesh sizes. Moreover, our optimization might produce different splitting of tolerance between bias and statistical errors than values traditionally used in MLMC. We present numerical results which highlight the functionality of the optimization by applying our method to an elliptic PDE with stochastic coefficients. We will emphasize how the optimal hierarchies change from the standard MLMC method as you include the effects of real problem parameters, such as the solver cost exponent.

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### CP7

### Estimation of Multi-Level Extrapolation Confidence

When system-level tests are unavailable, analysts calibrate the system model parameters using component-level tests and propagate the results to predict system performance. This presentation characterizes this extrapolation across levels using global sensitivity analysis and estimates the extrapolation confidence by comparing its sensitivity vector with that of a perfect extrapolation. The proposed approach facilitates selection of data sources and combination of activities for uncertainty quantification.

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### $\mathbf{CP7}$

### Multilevel MCMC/SMC Sampling for Inverse Electromagnetic Scattering

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 Bayesian inference can be performed by powerful multilevel SMC/MCMC methods, with estimates of material properties, hyperparameters and uncertainties.

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### CP7

### Multilevel Monte Carlo Methods with Control Variate for Elliptic SPDEs

We consider the numerical approximation of the stochastic Darcy problem and propose to use a Multilevel Monte Carlo approach combined with a control variate variance reduction technique on each level. The control variate is obtained starting from the solution of an auxiliary regularized problem and its expected value is computed with a Stochastic Collocation method on the finest level in which it appears. Numerical examples and a comparison with the <u>Francesco Tesei</u> ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE francesco.tesei@epfl.ch

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### CP7

### Multilevel Monte Carlo Simulations with Algebraically Constructed Coarse Spaces

We consider the numerical simulation of multiscale multiphysics phenomena with uncertain input data in a Multilevel Monte Carlo (MLMC) framework. Multilevel Monte Carlo techniques typically rely on the existence of hierarchies of computational meshes obtained by successive refinement. We apply MLMC to unstructured meshes by using specialized element-based agglomeration techniques that allow us to construct hierarchies of coarse spaces that possess stability and approximation properties for wide classes of PDEs. An application to subsurface flow simulation in mixed finite element setting illustrates our approach. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

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### CP8

### Uncertainty Quantification in Nanowire Sensors Using the Stochastic Nonlinear Poisson-Boltzmann Equation

We quantify fluctuations and noise in nanowire bio- and gas sensors using stochastic nonlinear and linear Poisson-Boltzmann equations. Random binding and unbinding of molecules and their movements are modeled as changes in permittivity and charge concentration. We have implemented various numerical methods such as Monte Carlo, quasi Monte Carlo, stochastic collocation, and stochastic Galerkin for the linear and the nonlinear equations, and we report on their relative performance. We also calculate the current through the sensors and compare it with measurements, finding that the nonlinear equation is much more realistic than the linear one.

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### CP8

#### Dissipative 2D Structures in Quintic Ginzburg Landau Equation

In this talk we examine the influence of parameters on the spatiotemporal solitons of 2D complex Ginzburg-Landau equation (CGLE) with cubic and quintic nonlinearities. The CGLE is solved numerically using a pseudospectral method with explicit RK4 time stepping. Numerical simulations, varying the system's parameters and initial conditions, reveal 2D solitons in the form of stationary, pulsating and exploding solitons with very distinctive properties. For certain regions of parameters, we have also found stable coherent structures in the form of spinning (vortex) solitons which exist as a result of a competition between focusing nonlinearities and spreading while propagating through medium.

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### $\mathbf{CP8}$

### The Effects of Design Uncertainties on Multiple Order Step Etalon Spectrometers

Multiple order etalon spectroscopy is a technique for building compact, low power spectrometers. These devices consist of a series of optical cavities, of varying length, sandwiched between two partial reflectors. These measurements can be used to recover the input spectrum. However, signal recovery from these measurements is very sensitive to the device design parameters. In this presentation we will present a sensitivity analysis of the proposed signal recovery algorithms with respect to these device parameters.

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#### $\mathbf{CP8}$

### First Order k-th Moment Analysis for the Nonlinear Eddy Current Problem

This paper is concerned with the stochastic nonlinear eddy current problem. The uncertainties of the magnetic fields or quantities of interest are studied in terms of the k-th moment and a first order Taylor expansion. In contrast to prior works, emphasis is put on uncertainties in the nonlinear magnetic material law. The approximation properties are mathematically analyzed and numerically verified by realistic examples.

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### CP8

### Searching Chemical Spectroscopy Libraries

Determining molecular compound identity is the central task of chemical analysis. It is often accomplished by comparing a spectrum of an unknown compound to a large library of spectra of known compounds. Traditionally chemical spectra are cast as vectors and a dissimilarity measure based on the inner product between known and unknown compound spectra is employed to determine a 'best match'. However, as libraries become larger, as the variety of instrument types grows, and as conditions change under which spectra are acquired, this measure of dissimilarity becomes far less effective at identifying unknowns. In this talk we describe various multidimensional scaling methods that go beyond the traditional library search techniques employed by chemists.

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### CP9

### Calibration and Confidence Assessment of Transient, Coupled Models Using Dynamic Bayesian Networks

Quantifying the uncertainty in transient response predictions for coupled systems is challenging in many applications. This presentation addresses calibration and confidence assessment for transient, coupled analyses using dynamic Bayesian networks. Time-dependent data are incorporated into the network to calibrate uncertain parameters and model discrepancies through time. A model reliability metric is used to assess the spatial and temporal confidence in the calibrated model predictions. The proposed methodology is illustrated with aerothermal models for hypersonic aircraft.

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### $\mathbf{CP9}$

#### Variational Bayesian Approximations for Nonlinear Inverse Problems

Bayesian formulations represent one of the prominent approaches for addressing problems of model calibration. Ex-

isting Bayesian methodologies are hampered by the highdimensionality of unknown model parameters and the high computational cost for inference. The present paper advocates a Variational Bayesian inference engine which exploits derivative information available from deterministic adjoint formulations. Furthermore we propose sparsityenforcing priors that are suited for spatially-varying model parameters and a greedy algorithm for learning the associated basis set.

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### CP9

### Bayesian Experimental Design for Stochastic Kinetic Models

In recent years, the use of the Bayesian paradigm for estimating the optimal experimental design has increased. However, standard techniques are computationally intensive for even relatively small stochastic kinetic models. One solution to this problem is to couple cloud computing with a model emulator. By running simulations simultaneously in the cloud, the large design space can be explored. A Gaussian process is then fitted to this output, enabling the optimal design parameters to be estimated.

### Colin Gillespie

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#### CP9

### Iterative Linear Bayesian Updating of Spectral Representations of Uncertainty

We present and discuss an iterative linear Bayesian uncertainty updating method based on spectral representations, with one example being Wiener's polynomial chaos expansion (PCE). The method can be seen as a tradeoff between linear and fully non-linear Bayesian parameter and state updating. It is aimed at bridging the gap between cheap, linear (or rather affine) methods and fully non-linear, expensive approaches. Connections to similar, random-sampling-based-methods such as the iterative ensemble Kalman filter are made.

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### CP9

### Solution of Inverse Problems with Limited Forward Solver Evaluations: A Bayesian Perspective

Solving inverse problems based on computationally demanding forward solvers is ubiquitously difficult since one is necessarily limited to just a few observations of the response surface. This limited information induces additional uncertainties on the posterior distributions. The main contribution of this work is the reformulation of the solution of the inverse problem when the expensive forward model is replaced by a set of simulations. We derive three approximations of the reformulated solution with increasing complexity and fidelity. We demonstrate numerically that the proposed approximations capture the epistemic uncertainty of the solution of the inverse problem induced by the fact that the forward model is replaced by a finite amount of data.

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### **CP10**

### Guarantees of Near-Optimal Experimental Input Design for System Identification

We introduce formal guarantees of near-optimal design of experiments aimed at system identification. In our scenario, the modeler can select interventions as control inputs to a nonlinear dynamical system. The objective is to maximize the statistical dependence, measured by mutual information, between models and data. We prove under which technical conditions this optimization problem exhibits properties for which near-optimal inputs can be selected in a polynomial number of evaluations of the objective.

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### **CP10**

### Generation of Uncertainty-Based Analytics for Selected Problems in Aerospace Systems Technology Transition

At the U. S. Air Force Research Laboratory, sensitivity analysis and uncertainty quantification assessments are critical activities that accelerate transition of innovative aerospace system technology in a budget-constrained fiscal environment. Uncertainty-based analytics are generated for program managers based on data sources that include reduced-order physics-based models, higher-fidelity models that require high-performance computing resources, experimental data, and flight test data. Results from implementation of a non-deterministic work flow are summarized for external aerodynamic case studies. We discuss organizational and resource challenges identified during implementation of this work flow, and provide suggestions on how to overcome these challenges to justify resource management.

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### **CP10**

### Enhanced Predictive Capability of Surrogate Models Through Model Selection

Surrogate models, such as cluster expansions, are generally challenged when predicting and optimizing properties learned from limited, noisy, data such as thermophysical quantities in metallic alloys. When coupled to, e.g., Monte Carlo sampling, the success of a subsequent property optimization, in the form of solving a complex model selection problem, hinges on robust, more advanced, inference techniques than currently employed. We show how reversible jump Markov Chain Monte Carlo techniques and relative entropy can remedy many of these important issues. Uncertainties airing from noisy data obtained from Molecular Dynamics simulations and the selection of parameters in the surrogate model are addressed and quantified.

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### **CP10**

### Design of Polynomial Chaos Basis for Sparse Approximation of Stochastic Functions

Conventionally, polynomial chaos (PC) bases are constructed with respect to the probability measure of random inputs. However, for arbitrary stochastic functions, these choices of bases may not lead to sparse/compact representations. In this work, we design an optimal PC basis within the Jacobi family that enhances the sparsity and accuracy of the standard PC expansion. Numerical tests will be provided to discuss the performance of this approach.

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### **CP10**

### Pc-Kriging: the Best of Polynomial Chaos Expansions and Gaussian Process Modelling

Polynomial chaos (PC) expansions and Kriging have emerged as powerful tools for uncertainty quantification, e.g. for sensitivity or reliability analysis. Interestingly, the two communities have little interaction. We show here how the two worlds may be combined at best using a type of universal Kriging in which the regression part is a sparse PC expansion. The optimal combination is investigated using Latin hypercube experimental designs and the results are compared in terms of achieved mean-square error, using either "pure PC', Kriging, or an optimal PC-Kriging surrogate.

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### **CP10**

#### Multi-Fidelity Wavelet Regression.

We study the prediction of an output produced by slow and complex simulator  $f_Y$  when we have access to less precise but faster versions, or levels, of  $f_Y$ . We propose a method in which we use an adaptive corase-to-fine wavelet decomposition. We select the wavelet coefficients to learn each level and the differences between them and to choose where and in which level, we should add new training points.

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### CP11

### A Model Reduction Algorithm for a Class of Stochastic Configurations

We consider absorption and scattering of acoustic waves from uncertain stochastic configurations comprising multiple bodies with various material properties and develop tools to address the problem of quantifying uncertainties in the acoustic cross sections of the configurations. The uncertainty arises because, for example, the locations and orientations of the particles in the configurations are described through random variables, and statistical moments of the far-fields induced by the stochastic configurations facilitate quantification of the uncertainty. In this talk we discuss an efficient model reduction algorithm to simulate the statistical properties of the stochastic model. We demonstrate the efficiency of the algorithm for configurations with nonsmooth and non-convex bodies with distinct material properties, and random locations and orientations with normal and log-normal distributions.

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### CP11

### Goal-Oriented Error Estimation for Reduced Basis Method

The reduced basis method is a powerful model reduction technique designed to speed up the computation of multiple numerical solutions of parameterized partial differential equations. We consider a quantity of interest, which is a linear functional of the PDE solution. We propose an efficiently, explicitly computable surrogate model error bound, and show on different examples that this error bound is sharper than existing ones. We include application of our work to sensitivity analysis studies.

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### **CP11**

### Stabilized Projection-Based Reduced Order Models for Uncertainty Quantification

Projection-based model reduction is a promising tool that can address the computational issues associated with UQ. Stability, accuracy, robustness, and efficiency are required for ROM to be viable. This talk focuses on a new approach for stabilizing ROMs that moves the unstable eigenvalues of a ROM system into the stable half of the complex-plane through the solution of an optimization problem. Various applications are discussed.

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#### **CP11**

### **Bayesian Reduced-Basis Models**

This paper deals with the development of probabilistic reduced-order models for systems with large number of input parameters in view of applications in uncertainty quantification. Existing reduced basis techniques assume that the solution can be approximated on an appropriately selected hyperplane. We advocate a Bayesian mixture of reduced-basis models on an inferred partition of the input parameter space and with appropriate sparsity-enforcing priors for automatically discovering the inherently dimensionality of the approximating hyperplanes.

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### CP11

### Optimal Reduced Basis for Vector-Valued Stochastic Processes Defined by a Set of Realizations

The use of reduced basis has spread to many scientific fields to condense the statistical properties of stochastic processes. Among these basis, the classical Karhunen-Loève basis plays a major role as it allows us to minimize the total mean square error. This paper presents therefore two adaptations of this Karhunen-Loève expansion to characterize optimized projection basis for stochastic processes that are vector-valued and only characterized by a relatively small set of independent realizations.

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### $\mathbf{CP12}$

### Fuzzy Risk Analysis Based on Ranking Fuzzy Numbers

Ranking fuzzy numbers plays a very important role in linguistic decision-making and some other fuzzy application systems. The last decades have seen a large number of methods investigated for fuzzy risk analysis based on ranking fuzzy numbers. The most commonly used approached is based on centroid points. However, there are some weaknesses associated with these indices. In this paper, we introduce an approximate method for ranking of fuzzy numbers based on the centroid point.

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### **CP12**

### Building Metamodels for Stochastic Simulation Codes

We present new metamodels adapted to stochastic numerical simulators, whose inputs are random variables and outputs are not scalar variables but probability density functions (pdfs). To emulate conditional pdfs in function of the simulator input variables, we propose two kinds of metamodels. The first one is based on a classical kernel regression method involving Hellinger distance between pdfs, while the second one aims at building a functional basis to approximate the learning sample of pdfs.

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### **CP12**

### Stochastic Multi-Disciplinary Analysis under Data Uncertainty and Model Error

This paper presents a probabilistic framework to include both aleatory and epistemic uncertainty in coupled multidisciplinary analysis (MDA). In the presence of natural variability, data uncertainty and model uncertainty, the methodology estimates the PDF of the coupling variables and subsystem/system level outputs that satisfy interdisciplinary compatibility. Global sensitivity analysis is extended to quantify the contributions of the uncertainty sources in such system. A mathematical MDA problem and an electronic packaging application are used for demonstration.

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### **CP12**

### An Origin of Macroscopic Uncertainty/randomness

The basic ideas of the so-called Clean Numerical Simulation (CNS) are described. The CNS is a parallel algorithm based on an arbitrary order Taylor series with an arbitrary precision of data. Thus, unlike other numerical algorithms, the CNS can reduce the numerical noises to such a low level that one can accurately simulate the propagation of physical uncertainty at micro-level. Using chaotic motion of three-body as an example, we illustrate that the micro-level physical uncertainty transfers into macroscopic uncertainty. Thus, the micro-level physical uncertainty is one origin of macroscopic uncertainty.

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### **CP12**

### Application of the Polynomial Chaos Technique for Global Sensitivity Analysis in a Finite Element Model for Deep Brain Stimulation

Deep brain stimulation (DBS) is a procedure to treat symptoms of motor skill disorders. Computational models of the brain are used to predict the extent of neural activation during DBS. We implemented a non-intrusive polynomial chaos technique in combination with Sobol' decomposition to perform a global sensitivity analysis in a human DBS model for several model parameters subject to uncertainty. Numerical integration methods based on tensor and sparse grids are compared regarding convergence and efficiency.

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### **CP13**

### Multi-Objective Well Placement Optimization under Geological Uncertainty

Uncertainty quantification is critical to oil and gas field development. This work develops a new workflow of well placement optimization process under geological uncertainty. We use multi-objective optimization techniques and consider both mean and variance of net present value for all geological realizations to obtain robust solutions. Coarse scale reservoir models are built for large fields to save simulation time. This workflow significantly increases the robustness of the optimization algorithm and enhances the computational efficiency.

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### **CP13**

### Investigation of Level Crossings in a Vertical Axis Wind Turbine (VAWT) using Probability Density Evolution Method (PDEM)

Stall flutter oscillations in synergy with external fluctuations can lead to the failure of a VAWT through multiple crossings over the threshold. Current work investigates the leverage of gust and flow uncertainties on such crossings. While Monte Carlo Simulations are inefficient, the Polynomial Chaos Expansion method is inaccurate, as it cannot simulate irregular response surfaces encountered in the analysis. However, PDEM, which uses the probability conservation principle, gives efficient and accurate results and is investigated currently.

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### **CP13**

### Emulation of Complex Simulator Models with Application to Hydrology

To reduce evaluation times of a general dynamic simulator, we construct its stochastic approximation, taking into account simulation mechanisms, named mechanismbased emulator. We quantify its precision gain over a non-mechanistic emulator. As an emulator prior, a time evolving state space model with a Gaussian processes as the innovation terms is used. We newly develop this technique for a continuous state space model and investigate its benefits on a case study from the field of hydrology.

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### **CP13**

### Uncertainty Propagation in Turbidity Currents Simulation

In this talk we address we deal uncertainties impact on the predictions originated from finite element models of sediment deposition by Turbidity Currents. We consider uncertainties in the initial conditions and in the deposition velocity as well. We use sparse grid stochastic collocation methods and particular attention is devoted to the construction of (multi point) statistics of the spatial deposition map.

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### CP13

### Polynomial Chaos Expansion for Subsurface Flows with Uncertain Soil Parameters

The effects of uncertain parameters in hydrological laws are considered in one-dimensional infiltration problems. Global sensitivity analyses quantify the influence of the variability of each input parameter on the position and the spreading of the wetting front. A Polynomial Chaos expansion with a non-intrusive spectral projection is used. Test cases with different laws are presented and demonstrate that second order expansions are well-adapted to represent h.bijl@tudelft.nl our quantities of interest.

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### **CP13**

### Reliability-constrained Robust Design Optimization for Multi-reservoir River Systems

The robust design objective formulation utilizes a weighted combination of the mean and variance of the performance function. We apply Stochastic Collocation to approximate a Certainty Equivalent from Utility Theory which allows efficient gradient computations. We then recycle collocation points to inform a surrogate of constraint functions which is used in a First Order Reliability Method. The combined approach is applied to a multiple dam hydro-power revenue optimization problem with uncertain inflows.

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### **CP14**

### Reconstructing Incompressible Flow Fields by Using a Physics-Based Covariance Model for Gaussian Processes

We manipulate the covariance of a Gaussian process model to enforce the mass continuity equation in the reconstruction of incompressible flow fields obtained from experimental data. By exploiting the Toeplitz-like structure of the gain matrix for measurements on a regular grid, we are able to make the method computationally feasible for large data sets. We apply the method to an experiment and show that the acquired field is incompressible and better able to reconstruct vortices.

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### **CP14**

### Non-Intrusive Polynomial Chaos Method in Hypersonic Scramjet Intake Flow

Scramjets are hypersonic airbreathing engines that utilize the unique technology of supersonic combustion. To quantify the uncertainty of the incoming flow a non-intrusive Polynomial Chaos method is used in combination with the in-house finite volume flow solver QUADFLOW. Since the inflow conditions during experiments and real flight are not constant, the inflow Mach number and the angle-of-attack are considered as aleatory uncertainties, and their impact on e.g. the wall pressure distribution is investigated.

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### **CP14**

### Deterministic Sampling for Uncertainty Quantification in Computational Fluid Dynamics

The Deterministic Sampling method is applied to an example of Uncertainty Quantification in Computational Fluid Dynamics (CFD). The high efficiency of DS is a game changer since CFD simulations are computationally intensive. The number of samples must be held to an absolute minimum in order have a feasible method for uncertainty quantification. Different sampling strategies will be presented which describe the uncertain parameter statistics with variable, but controllable balance between accuracy and ensemble size.

Peter Hedberg

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#### **CP14**

### Incompressible Navier-Stokes Equations with Stochastic Viscosity

A new stochastic Galerkin formulation of the incompressible Navier-Stokes equations is presented. The zero velocity divergence condition is replaced by a pressure Poisson equation. Stochastic viscosity is investigated, but the framework generalizes to general sources of uncertainty. We perform analysis to prove well-posedness. We devise a numerical method based on finite difference operators on summation-by-parts form that leads to time-stability with suitable boundary conditions and weakly enforces zero divergence of the velocity field.

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### **CP14**

### Tuning a RANS k-e Model for Jet-in-Crossflow Simulations

We develop a novel Bayesian calibration approach to address the problem of predictive k-e RANS simulations of jet-in-crossflow. We calibrate to experimental measurements of flow over a square cylinder. We estimate three parameters for the k-e model, by fitting polynomial surrogates of 2D RANS simulations to experimental data. The calibrated parameters seed an ensemble of 3D jet-incrossflow simulations. Our calibration delivers a significant improvement to the predictive skill of the 3D RANS model.

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### **CP14**

### Numerical Evaluation of a Parallel Stochastic Galerkin Solver for the Steady Incompressible Navier-Stokes Equations with Random Parameters

We evaluate numerically a parallel stochastic Galerkin multilevel method using Polynomial Chaos for the solution of the steady incompressible Navier-Stokes equations with random parameters. The parallelization is based on a domain decomposition for the spatial variable and a sharedmemory approach for the computation of the stochastic Galerkin residuals. We evaluate the multilevel method by solving the flow over a backward-facing step problem and the three-dimensional Lid-driven cavity with focus on convergence properties and computational time.

### Michael Schick

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### CP15

Quasi Monte Carlo Sample Selection for Depen-

### dent Uncertainty Spaces

In this talk, we present a computational method for selecting low-discrepancy points natively on a dependent space. This extends Quasi-Monte Carlo sampling techniques to spaces that are not equivalent to a hypercube. We derive a Koksma-Hlawka inequality that is customized to the dependent space, and pose sample selection as a binary quadratic program. We also present an efficient approximation algorithm based on the semi-definite programming relaxations for the MAX-CUT/BISECTION problems of graph theory.

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### CP15

### Sharp Asymptotic for the Pick Freeze Estimation of the Sobol Indices

The so-called Sobol indices quantify the energy of the Hoeffding factors in the orthogonal decomposition of a highly complex function. The function models a complicated input-output relationship. In this non linear regression model, the pick freeze method is a clever random sampling scheme that transforms the statistical estimation of the Sobol indices in a simple linear regression problem. In this talk, we will provide sharp non asymptotical results for these pick freeze estimators. Furthermore, we will discuss a natural multidimensional or functional extension of the Sobol indices as well as the properties of their pick freeze estimation. This conference will summarise some joint works developed with researchers of the Costa Brava project, http://www.math.univ-toulouse.fr/COSTA\_BRAVA/doku.php?id=index

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#### **CP15**

### Deterministic Sampling for Efficient and Accurate Quantification of Uncertainty

Deterministic sampling methods calculate model samples with definite rules for optimal performance. Their unprecedented efficiency and simplicity allow for uncertainty quantification of models of highest complexity, e.g. FEM and signal processing models. Deterministic ensembles are welldefined and thus possible to identify from reference data. The presentation will review our unique concept of deterministic sampling targeting optimal uncertain modeling. It includes methods for direct as well as inverse uncertainty quantification and comprises stratification and sample optimization.

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### CP15

### Randomized Pick-Freeze for Sparse Estimation of Sobol Indices in High Dimension

Sensitivity analysis is often performed by computing Sobol indices with respect to each input parameter (or group of input parameters). Classical estimation methods for these indices seem not very well suited for high-dimensional functions (functions with a large number of inputs). Besides, these functions often display sparsity of effects, i.e., a small number of inputs are influent. We propose an efficient, implementable and rigorously justified method to estimate Sobol indices in such contexts.

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### CP15

### Estimation of the Sobol Indices in a Linear Functional Multidimensional Model

We consider a functional linear model where the explicative variables are known stochastic processes taking values in a Hilbert space, the main example is given by Gaussian processes in  $\mathbb{L}^2([0, 1])$ . We propose estimators of the Sobol indices in this functional linear model. Our estimators are based on U-statistics. We prove the asymptotic normality and the efficiency of our estimators and we compare them from a theoretical and practical point of view with classical estimators of Sobol indices based on the Pick and Freeze scheme.

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### **CP16**

### First Passage Time for Uncertainty Quantifiaction of Numerical Environmental Models

Full knowledge of prediction error statistics of each numerical environmental model (such as numerical weather/ocean prediction model) is needed. Due to high structural complexity and high dimensionality of error phase space, establishment of such statistics is difficult. Usually the Gaussian distribution is assumed for the error statistics for simplicity. However, it might not be true. A scalar with the dimension of time, first-passage time (FPT), is defined as the time period when the prediction error first exceeds a pre-determined criterion (i.e., the tolerance level) is introduced to quantify the model uncertainty for linear and nonlinear stages in the prediction error evolution. The probability density function of FPT satisfies the backward Fokker-Planck equation Great advantages of FPT is also presented.

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### **CP16**

### A Chaotic Model for Bird Flocking

Pidgeons may be observed to flock in models that approximate the Lorenz Attractor. We would like to propose a model that is easily observable and exactly controllable, given certain parameters, for a flock of birds. Flocking is supposed to be controlled by three rules: separation, alignment, and cohesion. Are these the same rules that govern the behavior of the Lorenz Attractor? If so, we could conceive of discrete applications and continuous applications of this model. Discrete applications occur in graph theory and network theory; whereas continuous applications occur in flow theory. Indeed, the Lorenz Attractor was derived from a set of simplified Navier-Stokes equations, which govern flow. After looking at the examples, we then compare and contrast the flocking rules to the simplified Navier-Stokes equations.

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### CP16

### Multiple Patient Modeling over Bidimensional Riemannian Manifolds

A new approach to modeling spatially distributed data across several non-planar domains is developed to investigate the roles that hemodynamic forces and vessel morphology play in the pathogenesis of aneurisms. A generalized additive model that accounts for the complex geometry of each domain is extended to a multiple patient model by incorporating (space-varying) common and patient specific effects. This method merges Statistical and Numerical techniques to reduce the dimension of the problem and to solve the system.

### Bree Ettinger

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### **CP16**

### Constructing the Energy Landscape for the Gene Regulatory Network with Intrinsic Noise

Genetic switching driven by noise is a fundamental cellular process in genetic regulatory networks. With the autoregulatory dimer model as a specific example, we design a general methodology to quantitatively understand the metastability in gene expressions perturbed by the intrinsic noise based on the large deviation theory. Our approaches include the construction of quasi-potential energy landscape and the new large deviation result for the considered system.

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### **CP16**

### Validation and Uncertainty Quantification for Macroscale Soft Tissue Constitutive Models

We discuss the use of a Bayesian approach to calibrating and validating soft tissue constitutive models that are widely used in biomedical and biomechanical applications. We focus our attention on quantifying uncertainties in macroscopic constitutive models of soft tissue and propagate these uncertainties to simulations of soft tissue response. In particular we emphasize continuum constitutive models based on hyperelasticity and damage mechanics. The modeling is supported by synthetic and real experimental data from uniaxial extension and tearing experiments.

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### **CP17**

### Post-Optimality Analysis of Steel Production and Distribution

This study investigates the effect of uncertainty on the optimal production levels of steel production problem formulated as LP. The steel company distributes its products to several markets. Variations in problem parameters such as prices, supply, and demand can affect the profitability. Herein, stability limits, within which the obtained solution remains optimal, are calculated. The results identify sensitive parameters that need accurate estimate or extensive monitoring; and where sensitivity information, Lagrange multipliers, are valid.

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### **CP17**

### Bayesian Network Identification of Thermal Buckling in Thin Beam Experiments

Bayesian networks are a beneficial paradigm for understanding a system and model uncertainty, natural variability, and experimental error. In this study, a Bayesian network was constructed from experimental and model data to identify the buckled state from thermally-loaded, clampedclamped thin beams. From the observed natural frequencies and temperatures, a Bayesian network was trained to identify whether the beam was buckled or unbuckled. In addition, sensitivity analysis was performed, and the critical buckling temperature was estimated.

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### **CP17**

### Uncertainty Quantification of Manufacturing Process Effects on Material Properties

This presentation discusses uncertainty propagation from manufacturing process to material microstructure to macro-level properties. Simulation of cooling down process was introduced, during which microstructure would be gradually formed. Based on the generated microstructure, macro-level properties could be predicted via homogenization method. Gaussian Process surrogate model was built to show how certainties of material properties are affected by uncertainties of microstructure initial conditions as well as environment changes.

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### **CP17**

### Bayesian Calibration of Thermal Buckling Models for Thin Panels

Accurately estimating the prestress induced by the assembly of thin panels on future hypersonic aircraft is critical for determining the buckling load from computational models. Natural frequency and temperature test data from thermally-loaded, clamped-clamped thin beam specimens was used for Bayesian model calibration of uncertain system parameters, including the prestress. Validation data was used to assess prediction confidence for the computational model.

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### **CP17**

### Identifying Sources of Model Uncertainty in Hypersonic Aerothermoelastic Predictions

The inherently multi-physics nature of hypersonic aircraft structural response requires coupled models to capture the fluid-thermal-structural interaction. To enable model selection and uncertainty reduction, it is essential to understand the contribution of model uncertainty from the individual components in the aerothermoelastic system. This research investigates the identification of model form error in aerodynamic pressure and heat flux predictions, as well as solution approximation error in nonlinear reduced order Benjamin P. Smarslok Air Force Research Laboratory benjamin.smarslok@us.af.mil

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### **CP18**

### Inverse Problems and Uncertainty Quantification: Low-Rank Matrix Inverse Approximations

Oftentimes, the desired solution of an inverse problem can be well-represented using only a few vectors of a certain basis, e.g., the singular vectors. We design an optimal low-rank matrix inverse approximation by incorporating probabilistic information from training data and solving an empirical Bayes risk minimization problem. We focus on how the computed low-rank inverse approximation can be used to provide improved solution estimates and computable estimates of the uncertainty in our solutions.

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### **CP18**

### Non Intrusive Galerkin Method for Solving Stochastic Parametric Equations in Low-Rank Format

We propose to revisit classical algorithms for solving stochastic parametric equations using Galerkin spectral methods in a non intrusive fashion. We rely on the projection of a numerical scheme for computing an approximation of the parametric solution, which requires the evaluation of samples of the iteration map. The method is extended to the computation of a low-rank approximation of the solution, with the evaluation of samples of the residual.

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### **CP18**

### Dynamical Low Rank Approximation of Time Dependent Pdes with Random Data

We propose a Dynamically Orthogonal Field (DOF) approach to solve time dependent partial differential equations with random input data. The objective is to approximate the solution depending on the physical variable and the random parameters in a manifold of low dimension  $\mathcal{M}_s$  of functions in separable form. This is obtained by projecting at each time step the residual of the governing equation onto the tangent space to  $\mathcal{M}_s$  at u(t). Under suitable conditions, it is shown that the error of the DOF approach can be bounded in terms of the best approximation error.

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### **CP18**

### Low-Rank Solution of Unsteady Diffusion Equation with Stochastic Coefficients

The discretization of unsteady diffusion equation with random inputs using the stochastic Galerkin finite element method generally yields large linear systems with Kronecker product structure. Hence, solving them can be timeand computer memory-consuming. First, we show that the solution of such systems can be approximated with a vector of low tensor rank. Next, we solve them using low-rank preconditioned iterative solvers. Numerical experiments demonstrate that these solvers are quite effective.

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#### **CP18**

### Variance Reduction Based $l_1$ -Minimization Methods for Sparse Approximation of Stochastic Partial Differential Equations

We approximate solutions of stochastic PDEs with polynomial chaos expansion using  $l_1$ -minimization combined with a variance reduction method. We construct a reduced-order model from a small set of samples to reduce variance of the remaining samples. We use the samples with reduced variance to approximate the solution using  $l_1$ -minimization. This methodology is useful when the variance of the solution is high and available samples are limited.

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### **CP18**

#### Goal-Oriented Low-Rank Approximations for High Dimensional Stochastic Problems

We propose a minimal residual method for the solution of high dimensional equations using low-rank tensor formats. The measure of the residual is such that the resulting approximation is quasi-optimal with respect to a specified distance to the solution. This distance is chosen such that the optimality of the approximation is achieved with respect to some quantity of interest that can expressed as a linear form of the solution. The resulting method can be seen as an optimal goal-oriented model reduction method.

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#### MS1

### Iterative Solution of Reduced-Order Models for Parameter-Dependent PDEs

One way to reduce computational costs associated with PDEs depending on large numbers of random parameters is through reduced basis methods. These methods attempt to represent the system using a small number of realizations of solutions, the reduced space, such that other realizations can be approximated well in the reduced space. If the dimension of the reduced space is much smaller than that of the discrete PDE, then it will cheaper to use straightforward algebraic techniques to find solutions in the reduced space than in the full discrete space. However, it may be that the reduced space is small relative to the full discrete space but the cost of direct methods for reduced solution is higher than that of fast methods such as multigrid for the full system. In this study, we explore iterative methods for the reduced problems and show that when the number of parameters is large, they are more effective than standard algebraic approaches.

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### ${\bf MS1}$

### Coherence Motivated Monte Carlo Sampling of Sparse Polynomial Chaos Bases

We investigate Monte Carlo sampling of random inputs for the estimation of coefficients in a sparse polynomial chaos expansion, with a particular focus on high-dimensional random inputs. Sampling from the distribution of the random variables is typically sub-optimal in a statistical sense. Asymptotic properties of orthogonal polynomials yield sampling schemes with reduced dependence on the order and dimension of polynomial basis. We present alternative sampling schemes, particularly for Hermite and Jacobi polynomial approximations, including a Markov Chain Monte Carlo sampling with a statistical optimality.

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### $\mathbf{MS1}$

### Optimal Polynomial Approximation of Elliptic PDEs with Stochastic Coefficients

We analyze the convergence of the Stochastic Galerkin and Stochastic Collocation methods based on multivariate polynomials for the numerical solution of PDEs with random inputs. We present strategies to construct optimal spaces and propose some particular polynomial spaces and generalized sparse grids that are optimal for particular problems. We discuss the convergence rate of these methods in arbitrary dimension depending on the number of PDE solves. We also illustrate our results with numerical examples.

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#### MS1

### A Generalized Clustering-based Stochastic Collocation Approach for high-dimensional Approximation of PDEs with Random Input Data

We developed a novel generalized clustering-based stochastic collocation (gSC) approach, constructed from, e.g., a latinized hCV tessellation (hCVT), with locally supported hierarchical radial basis function defined over each hCVT cell. This gSC method permits low-discrepancy adaptive sampling according to the input probably density function (PDF), and whose accuracy decreases as the joint PDF approaches zero; effectively approximating the solution only in the high-probability region. Theoretical and computational comparisons to classical sampling and SC methods will also be examined.

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#### MS2

Impacts of Varying Spatial and Temporal Density

### of Observations on Uncertainty with An Atmospheric Ensemble Prediction System

The Data Assimilation Research Testbed and the Community Atmosphere Model (DART/CAM), both developed at the National Center for Atmospheric Research, are used for ensemble Kalman filter observing system simulation experiments. The ability of observations taken at the earth's surface to constrain the entire depth of the troposphere is explored with a sequence of experiments. Both the spatial and temporal density of the observations is varied with a particular focus on very frequent observations.

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### $\mathbf{MS2}$

### Quantification of Bayesian Filter Performance for Complex Dynamical Systems through Information Theory

Practically implementable filtering/data assimilation strategies in high-dimensional dynamical systems are generally imperfect and not optimal due to computational constraints and the formidably complex nature of the underlying true dynamics. We exploit connections between information theory and the filtering problem in order to establish bounds on the filter error statistics, and to systematically study the statistical accuracy and utility of various Kalman filters with model error for estimating the dynamics of partially observed turbulent systems. The effects of model error on filter stability and accuracy in this high-dimensional setting are analyzed through appropriate information measures in the statistical 'superensemble' setting. Particular emphasis is on the notion of practically achievable filter skill which requires trade-off's between different facets of filter performance. This information-theoretic framework has natural generalizations to imperfect Kalman filtering with non-Gaussian statistically exactly solvable forecast models.

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### MS2

### Nested Particle Filters for Sequential Parameter Estimation in Discrete-time State-space Models

The problem of estimating the parameters of nonlinear, possibly non-Gaussian discrete-time state models has drawn considerable attention during the past few years, leading to the appearance of general methodologies (SMC<sup>2</sup>, particle MCMC, recursive ML) that have improved on earlier, simpler extensions of the standard particle filter. However, there is still a lack of recursive (online) methods that can provide a theoretically-grounded approximation of the joint posterior probability distribution of the parameters and the dynamic state variables of the model. In the talk, we will describe a two-layer particle filtering scheme that addresses this problem. Both a recursive algorithm, suitable for online implementation, and some results regarding its asymptotic convergence will be presented.

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### $\mathbf{MS2}$

### Accuracy and Stability of The Continuous-Time 3dvar Filter for The Navier-Stokes Equation

The problem of effectively combining data with a mathematical model constitutes a major challenge in applied mathematics. It is particular challenging for highdimensional dynamical systems where data is received sequentially in time and the objective is to estimate the system state in an on-line fashion; this situation arises, for example, in weather forecasting. The sequential particle filter is then impractical and *ad hoc* filters, which employ some form of Gaussian approximation, are widely used. Prototypical of these ad hoc filters is the 3DVAR method, with the extended Kalman filter (ExKF) and ensemble Kalman filter (EnKF) arising as important generalizations. In this talk we focus mainly on the accuracy and stability of 3DVAR filters for the Navier-Stokes equation We work in the high frequency limit and derive continuous time filters, that lead to a stochastic partial differential equation (SPDE) for state estimation, in the form of a damped-driven Navier-Stokes equation, with meanreversion to the signal, and spatially-correlated time-white noise. By studying the properties of this SPDE we deduce important information about the behaviour of the filter. We finish the talk by presenting various numerical simulations that illustrate our findings.

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### MS3

### Not available at time of publication

Not available at time of publication.

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### $\mathbf{MS3}$

### Multi-parameter Regularization via an Augmented Approach

In this talk, we revisit muti-parameter regularization from the perspective of augmented Tikhonov regularization. We shall discuss the Bayesian motivation within the hierarchical Bayesian framework. We derive novel parameter choice rules, e.g., balanced discrepancy principle. The efficient implementation of the rules are also discussed, and numerical results are given.

#### Bangti Jin

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### MS3

### Multi-Parameter Regularization for Lifting the Curse of Dimensionality

Inspired by the increased demand of robust predictive models, we present comprehensive analysis of techniques and numerical methods for performing reliable predictions from roughly measured high-dimensional data. Namely, we discuss the use of multi-penalty regularization in Banach spaces in high-dimensional supervised learning. We focus on two mechanisms of dimensionality reduction by assuming that our function has special representation/format and then we recast the learning problem into the framework of multi-penalty regularization with adaptively chosen parameters.

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### $\mathbf{MS4}$

#### Calibration in the Presence of Model Discrepancy

Unknown parameters in computer models may be of intrinsic scientific interest, so that learning about them is not only essential for prediction purposes but also contributes to the underlying science. It is well known that calibration analysis that does not account for model discrepancy will lead to biased and over-confident parameter estimates and predictions. However, incorporating model discrepancy is challenging due to the confounding with calibration parameters, which can only be resolved with meaningful priors. In this talk we illustrate the effect this confounding has on uncovering true physical parameters and discuss ideas for how to incorporate prior information to mitigate the problem.

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MS4 Parameter Calibration Accounting for Multiple

#### Sources of Modeling Uncertainty

Parameter calibration for differential equation models is difficult due to lack of uncertainty quantification in the model solution, model mis-specification, and the black box nature of the differential equation solver. In this talk we bring together insights and methods from the previous 3 talks in this session to show how the probabilistic state and derivative information fits into producing an emulator with a model discrepancy term to calibrate parameters.

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### MS4

### Building Better Simulators: Providing a Probabilistic Representation of Numerical Uncertainty in the Response

Computer simulators rely on discretization-based techniques to solve large-scale systems of differential equations. We incorporate systematic uncertainty due to discretization into a computer simulator via a probability model characterizing our knowledge of the solution by a probability measure on the phase space. We demonstrate our approach on the time and space evolution of states governed by the Navier-Stokes equations in the chaotic regime, where any unmodelled discretization error quickly becomes amplified.

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### MS4

### Model Calibration with Complex Differential Equation Constraints

Computer model calibration experiments enable scientists to combine simulators of real-world processes with observational data to form predictions and solve inverse problems. Gaussian Processes are a popular statistical model for calibration experiments, however the covariance function does not incorporate knowledge of the simulator, thereby misrepresenting uncertainties. We incorporate a simulators derivative information into a Gaussian Process calibration model, reducing uncertainties, improving predictive interval coverage and calibration parameter estimate accuracy, as demonstrated using a real-world problem.

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### $\mathbf{MS5}$

### Applications of Machine Learning to Climate Model UQ

From the execution of simulations on supercomputers to the exploration of high-dimensional parameter spaces, machine learning algorithms can play a powerful role in the quantification of uncertainties in climate models. Training data derived from perturbed physics-parameter ensembles are used to learn about uncertainties in the Community Earth System Model. We present cases using feature selection to determine sources of model variability, failure analysis to detect simulation anomalies, and supervised regression to perform model inversion.

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#### $\mathbf{MS5}$

### Assessing High-Dimensional Space and Field Dependencies Between Modeled and Observed Climate Data

The scientific, statistical, and computational strategies that are used for uncertainty quantification are key to the future of climate model development. The objective of this talk is to present strategies for better representing scientific sensibilities within statistical measures of model skill that then can be used within a Bayesian statistical framework for data-driven climate model development and improved measures of model scientific uncertainty. In particular we propose a statistical approach that can leverage HPC resources to help reduce biases in future versions of the NCAR Community Atmosphere Model (CAM). Specifically, we consider concepts from Gaussian Markov Random Fields (GMRFs) to create a multi-variate metric that takes into account spatial and field dependencies. We compare how this metric relates to more traditional strategies based on singular value decomposition and empirical orthogonal functions. We also compare how covariances of fields computed from GMRFs relate to data/observational covariances.

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### MS5

### Impact of Model Resolution for Regional Climate Experiments

Understanding the role of model resolution and the interaction with model components is becoming an increasingly important aspect of climate modeling. In this work, I will present an analysis of a regional climate model experiment focusing on monthly precipitation and understanding the interaction between model resolution and convective parameterizations. In addition, I will present a statistical framework for the analysis of the large datasets associated with climate model output.

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### MS5

### Joint Parameter Exploration of Land Surface and Atmospheric Response to Greenhouse Gas Forcing in Cesm1-Cam5

We present a new methodology for rapidly exploring the response surface of a high complexity GCM using a surrogate constructed using single point simulations of the same model. The methodology is demonstrated using the single point version of CESM1-CAM5, together with a small number of global simulations of the land and atmosphere models. In this study, we use idealized climate change experiments simulated at the point level in different climatic regimes to act as a predictor of large scale climate and carbon cycle response, and compare results to more traditional surrogate techniques. Candidate parameter configurations are proposed for optimized versions of the model at a range of global climate sensitivity and net carbon cycle response, which will be used in future to produce a small targeted perturbed ensemble using CESM1-CAM5.

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#### MS6

### Multiscale Filtering with Superparameterization

Observations of a true signal from nature at a physical location include contributions from large and small spatial scales. Most atmosphere and ocean models fail to resolve all the active spatial scales of the true system; 'parameterizations' attempt to diminish the model error associated with not resolving the small scales. However, in most filtering and data assimilation algorithms that use underresolved models the model variables are tacitly assumed to correspond to the physical values of the true variables rather than the large-scale part of the true variables. When the unresolved scales contribute a significant amount to the observations this incurs a large error because underresolved models only model the contribution of the large scales to the observations. We explore multiscale filtering algorithms that address this problem; in particular we focus on using superparameterization, a multiscale parameterization method, to both reduce large-scale model error and supply information on the unresolved scales.

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#### MS6

### Statistically Accurate Low Order Models for Uncertainty Quantification in Turbulent Dynamical Systems

A new framework for low order predictive statistical modeling and uncertainty quantification in turbulent dynamical systems is developed here. These new reduced order modified quasilinear Gaussian (ROMQG) algorithms apply to turbulent dynamical systems where there is significant linear instability or linear non-normal dynamics in the unperturbed system and energy conserving nonlinear interactions which transfer energy from the unstable modes to the stable modes where dissipation occurs, resulting in a statistical steady state; such turbulent dynamical systems are ubiquitous in geophysical and engineering turbulence. The ROMQG method involves constructing a low order nonlinear dynamical system for the mean and covariance statistics in the reduced subspace which has the unperturbed statistics as a stable fixed point and optimally incorporates the indirect effect of non-Gaussian third order statistics for the unperturbed system in a systematic calibration stage.

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### MS6

### Goal-oriented Probability Density Function Methods for Uncertainty Quantification

We propose a new framework for uncertainty quantification (UQ) in high-dimensional stochastic systems based on goal-oriented probability density function (PDF) methods. The key idea stems from techniques of irreversible statistical mechanics, and it relies on deriving evolution equations for the PDF of a low-dimensional quantity of interest, i.e., a functional of the solution to stochastic ordinary and partial differential equations. Numerical applications are presented for stochastic resonance and advection-reaction problems.

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### $\mathbf{MS6}$

### Modeling Uncertainty in Chaos and Turbulence Using Polynomial Chaos and Least Squares Shadowing

Uncertainty in simulations of chaotic systems lies in approximating physical models, limited simulation time, and discretizing broad temporal and spatial scales. The high computational cost of these simulations makes brute force UQ methods impractical. The chaotic dynamics leads to an ill-conditioned initial value problem whose extreme sensitivity prohibits the use of polynomial-based UQ methods. We introduce Least Squares Shadowing, a method that overcomes the ill-conditioning and enables polynomial methods to quantify the uncertainties.

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### $\mathbf{MS7}$

### Quantifying Uncertainties in Ice Sheet Paleo-Thermometry

Ice sheet temperature evolution is governed by internal heat generation, basal fluxes, and surface temperature. Reconstructed surface boundary conditions have been used as indicators of past climate variations. Quantifying uncertainty in these reconstructions can be difficult since surface temperature has infinite degrees of freedom correlated on a characteristic timescale, and the data do not equally constrain uncertainty at all points in time. State-of-theart uncertainty quantification tools are used to solve this problem in a framework easily extended to larger models with complex parameter spaces.

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#### MS7

### Representation of Thwaites Glacier Bed Uncertainty in Modeling Experiments

Not available at time of publication.

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### MS7

### Uncertainty Quantification for Large-Scale Bayesian Inverse Problems with Application to Ice Sheet Models

We consider the estimation of the uncertainty in the solution of (large-scale) ice sheet inverse problems within the framework of Bayesian inference. The posterior probability density is explored using an MCMC sampling method that employs local Gaussian approximations based on gradients and Hessians (of the log posterior) as proposals. We show inference results for the basal sliding coefficient from surface velocity observations and prior information and compare the performance of three Hessian-based MCMC sampling methods.

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### $\mathbf{MS7}$

### Sensitivity of Greenland Ice Flow to Errors in Model Forcing, Using the Ice Sheet System Model and the DAKOTA Framework

With use of established uncertainty quantification capabilities within the Ice Sheet System Model (ISSM), we compare the sensitivity of simulated Greenland ice flow to errors in various forcing, including surface mass balance, temperature, and basal friction. We investigate how errors propagate through the model resulting in uncertainties in ice discharge. This work was performed at the California Institute of Technology's Jet Propulsion Laboratory under a contract with the NASA's Modeling, Analysis and Prediction Program.

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### $\mathbf{MS8}$

### Model Calibration for Large Computer Experiments

Combining simulator output with field observations to make predictions for a system and estimate process parameters is called calibration. The traditional approach uses a Gaussian process to model various response surfaces. When the number of runs of the computer model is large, inference because computationally challenging. We propose a new approach to approximate the Gaussian process using local subsets of the data for model calibration. The methodology is motivated from the calibration of radiative shocks.

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### $\mathbf{MS8}$

### Optimal Bayesian Experimental Design in the Presence of Model Error

We propose an information theoretic framework and algorithms for robust optimal experimental design with simulation-based models, with the goal of maximizing information gain in targeted subsets of model parameters, particularly in situations where experiments are costly. Our framework adds calibration and/or discrepancy terms in order to "relax' the model so that proposed optimal experiments are more robust to model error or inadequacy. We illustrate the approach via several model problems and misspecification scenarios.

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#### MS8

### Efficient Inference Using Sparse Grid Experimental Designs

Recently, random field models have been widely employed to develop predictors of expensive functions based on observations from an experiment. In high dimensional scenarios, the traditional framework for analysis struggles due to the computational burden of inference. This work proposes a class of experimental designs that has two useful properties: (1) the designs allow for computationally efficient development of predictors and (2) the designs perform well in terms of prediction accuracy (even in high dimensions).

### <u>Matthew Plumlee</u> ISYE, Georgia Tech mplumlee@gatech.edu

### $\mathbf{MS8}$

### Bayesian Inference and Uncertainty Quantification for Computationally Expensive Models using High Dimensional Emulators

Bayesian inference and calibration for computationally expensive simulators is often complicated by the limited number of likelihood evaluations that are feasible. Our novel inference strategy, which uses dimension-reduced Gaussian process emulators of high dimensional simulator output, is less reliant on the determination of tuning parameters than previous approaches, and allows model diagnostics without requiring additional simulator evaluations. We demonstrate the methods through applications to simulators from the biological and pharmaceutical sciences.

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### MS9

### Dimension Dependence of Sampling Algorithms in Hierarchical Bayesian Inverse Problems

We will study properties of the Gibbs sampler used for sampling the posterior in certain hierarchical Bayesian formulations of linear inverse problems. Emphasis will be placed on the insight obtained from formulating the problem in function space and this insight will be used to understand the mixing behavior of the Gibbs sampler as the discretization level increases. Our methods also apply to a range of nonlinear inverse problems such as nonparametric SDE drift estimation.

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### $\mathbf{MS9}$

### Parallel Monte Carlo with a Single Markov Chain

Markov chain Monte Carlo methods are essential tools for solving many modern day statistical and computational problems, however a major limitation is the inherently sequential nature of these algorithms. In this talk we propose a natural extension to the Metropolis-Hastings algorithm that allows for parallelising a single chain using existing MCMC samplers, while maintaining convergence to the correct stationary distribution. We do so by proposing multiple points in parallel, then constructing and sampling from a finite state Markov chain on the proposed points that has the correct target density as its stationary distribution. Our approach is generally applicable, easy to implement, and particularly useful for introducing additional parallelisation for models that are expensive to compute. We demonstrate how this construction may be used to greatly increase the computational speed via parallelisation of a wide variety of existing MCMC methods, including Metropolis-Adjusted Langevin Algorithms and Adaptive MCMC. Furthermore we show how it allows for a principled way of utilising every integration step within Hamiltonian based MCMC methods, resulting in increased accuracy of Monte Carlo estimates with minimal extra computational cost.

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### $\mathbf{MS9}$

### Posterior Exploration of Inverse Equilibrium Problems Using a New a Gibbs-Like Sampler

The standard Gibbs sampler is equivalent to Gauss-Seidel iteration, when applied to Gaussian-like target distributions. This explains the slow (geometric) convergence, but also indicates how to accelerate using polynomials. The potential to accelerate prompts our interest in the Gibbs sampler for an application of capacitance tomography. We report a near-analytic Gibbs sampler in the broader class of inverse equilibrium problems derived by utilizing the graph-theoretic construction of circuit theory.

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### MS9

### Multilevel Markov Chain Monte Carlo with Applications in Subsurface Flow

We address the prohibitively large cost of Markov chain Monte Carlo for large-scale PDE applications with high dimensional parameter spaces. We propose a new multilevel Metropolis-Hastings algorithm, and give an abstract theorem on its cost. For a typical model problem in subsurface flow, we then provide a detailed analysis of the assumptions in the theorem and show gains of at least one order in the  $\varepsilon$ -cost over standard Metropolis-Hastings both theoretically and numerically.

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### $\mathbf{MS10}$

### Uncertainty Quantification of Errors from Reduced-Order Models

In many UQ settings, surrogate models are essential for reducing the cost of forward simulations. These surrogates are typically one of the following:

- 1. **Data fits** that yield statistical models of the quantities of interest, but lack robustness as they are 'blind' to underlying physics.
- 2. **ROMs** that are physics based, but lack a useful statistical interpretation: their rigorous error bounds often grossly overestimate the error and are not statistically useful.

We aim to combine the benefits of these approaches by correcting the ROM prediction via an efficient statistical data-fit model of the ROM error.

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### MS10

### Adaptive *h*-refinement for Nonlinear Reducedorder Models with Application to Uncertainty Control

Reduced-order models (ROMs) decrease the cost of forward simulations, but the model-form uncertainty they introduce is challenging to quantify and control. We therefore present an adaptive ROM refinement approach that applies ideas from h-adaptivity to low-dimensional bases. Refinement is achieved by generating a hierarchy of trial subspaces  $S_i \subset S_{i+1}$ , where  $S_{i+1}$  is computed from  $S_i$  via 'basis splitting' in two steps: 1) identify basis vectors to split, and 2) split each identified vector into two basis vectors with non-overlapping support.

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### $\mathbf{MS10}$

#### Reduced Basis Method and Several Extensions for Uncertainty Quantification Problems

We develop and analyze several extensions of reduced basis method (RBM) as a model reduction technique in solving UQ problems. In particular, a weighted RBM is proposed to incorporate the probability density function of the random variables in order to construct an efficient and accurate reduced basis space. We provide a priori convergence analysis of the proposed method and demonstrate its performance by several numerical experiments with high dimensional and low regularity properties.

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### MS10

### Reduced Basis Collocation Methods for Partial Differential Equations with Random Coefficients

The sparse grid stochastic collocation method is a new method for solving partial differential equations with random coefficients. However, when the probability space has high dimensionality, the number of points required for accurate collocation solutions can be large, and it may be costly to construct the solution. We show that this process can be made more efficient by combining collocation with reduced basis methods, in which a greedy algorithm is used to identify a reduced problem to which the collocation method can be applied. Because the reduced model is much smaller, costs are reduced significantly. We demonstrate with numerical experiments that this is achieved with essentially no loss of accuracy.

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### MS11

### Large Deviations for Stochastic Dynamical Systems Driven by a Poisson Noise

The goal of this work is to develop a systematic approach

for the study of large deviation properties of infinite dimensional systems driven by a Poisson noise. Our starting point is a variational representation for exponential functionals of general Poisson random measures and cylindrical Brownian motions. The representation is then used to give a general sufficient condition for a large deviation principle to hold for systems that have both Brownian and Poisson noise terms. Finally we give examples to illustrate the approach.

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### MS11

### Large Deviations and Variational Representations for Infinite Dimensional Stochastic Systems

We discuss how certain variational representations can be used to develop an efficient methodology for large deviations analysis, especially in the infinite dimensional setting. We first review their use in a simple setting, and then describe the form of the representation and its application to the infinite dimensional setting. If time permits moderate deviations and connections with Monte Carlo will be discussed.

### Paul Dupuis

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### MS11

### The Minimum Action Method for the Study of Rare Events

Many physical processes are driven by rare but important events. The presence of small noise in the system makes the system hop between metastable states, make excursions out of these states, etc. The large deviation theory gives an estimate on the probability of the paths in terms of an action functional. The most probable path is given by the one that minimizes the action functional. In the minimum action method, this is used as a numerical tool in which optimal trajectories between the initial and final states in the system are computed by minimizing the action functional. I will talk about the minimum action method and its applications to spatially extended systems including thermally activated reversal in the Ginzburg-Landau model and a barotropic flow over topography.

#### Weiqing Ren

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### MS11

### Efficient Computation of Instantons in Complex Systems

I will discuss several methods to compute minimizers of the Freidlin-Wentzell action in nonlinear systems. As a main example of the discussed methods I will present an application related to the stochastically driven Burgers equation and the quantification of the occurrence of shocks with large negative gradients in such systems.

### Tobias Schaefer

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### $\mathbf{MS12}$

### Quantification of Model Form Uncertainty for Run-Time Optimization of Simulation-Based Predictions

For some applications the optimal model–form to obtain a reliable prediction can also depend on its computational complexity. In this presentation we address applications where data to estimate the the uncertainty is only available for problem sizes far smaller than required by the predictive model. The computed uncertainty of the prediction model and its expected run–time therefore need to be extrapolated and balanced out. Motivation and test examples for this work are provided by SST/macro, a model that simulates software performance on unknown hardware architectures.

### Martin Drohmann

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### $\mathbf{MS12}$

### Calibration, Validation, and Model Uncertainty of Coarse-Grained Models of Atomic Systems

The predictability of coarse-grained (CG) approximations of atomistic systems is explored. We develop basic principles for developing CG and, eventually, macro-scale models based on Bayesian methods of statistical calibration and model selection, and information theory. Examples of molecular model calibration, determination of priors on parameters using minimum entropy principles, estimates of CG and continuous model bias, and validation processes for models of polymer chains and models of elastostatics of hyperelastic materials are described.

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### MS12

### **Options for Quantifying Model Form Uncertainty**

Different routes for quantifying model form uncertainty are investigated, based on calibration, verification and validation activities. These include Bayesian model calibration with a discrepancy term; estimation of various numerical errors and subsequent isolation of model form error; and expression of model form uncertainty through validation metrics. Different options within each route as well as their effects on quantifying the prediction uncertainty are investigated. The methods are illustrated with multi-physics, multi-scale application examples.

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### $\mathbf{MS12}$

### Multi-Fidelity Uncertainty Quantification of Complex Simulation Models

We investigate uncertainty quantification of simulation models based on training data of varying quality levels. The cheaper lower-quality data is corrected by a Bayesian process to produce a substitute for the expensive, sparse high-quality data. The process requires very few evaluations of the full-model, thus applicable to situations where sampling-based analysis is not possible. We provide the basic algorithm, and demonstrate on a flow model implemented using a high-fidelity fluid dynamics solver Nek5000.

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### $\mathbf{MS13}$

### Uncertainty Quantification in the Wind-Wave Model WaveWatch-III

Surface waves on the ocean are important not only for their scientific interest but also for safety at sea and the damage done to offshore and coastal structures. Numerical models of waves, such as WaveWatch III are complex; balancing the wind input, non-linear wave-wave interactions and wave dissipation. We analyse a series of models, from idealized zero dimension models, through 1-d to 2-d versions of the model, concluding with an implementation for Lake

Michigan.

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Ben Timmermans, Christine Gommenginger National Oceanography Centre ben.timmermans@soton.ac.uk, cg1@noc.ac.uk

### MS13

### High Performance Computation of Spatial Field Estimates

Estimation of spatial fields from samples is an essential operation in Earth system analysis, as in the generation of regional surface temperature fields given observation station data. We present challenges and prospects of methods for high-performance computation focusing on two approaches: Lattice Kriging extends covariance-based spatial statistical methods to model very large datasets; and Bayesian Additive Regression Trees, an unconventional spatial method that can handle massive data sizes in a highly-parallel framework. Spatial field predictions and uncertainty are compared.

<u>James Gattiker</u> Los Alamos National Laboratory gatt@lanl.gov

### MS13

### Simulating and Analyzing Massive Multivariate Remote Sensing Data

We present methods to simulate geophysical fields at different heights with heterogeneous correlation structure. With parameters calibrated using coarse-resolution climate model outputs, the multivariate statistical model enables us to simulate values with statistical characteristics consistent with scientific understanding. This multivariate simulation model incorporates dimension reduction and can generate values at high resolution. We will also discuss how to obtain optimal estimates and associated uncertainties of these geophysical fields simultaneously from multiple incomplete and noisy datasets.

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### **MS13**

### Computational Methods for Large Multivariate Spatio-Temporal Computer Model Outputs

In this talk, we consider computer models that have multivariate outputs that evolve in space and time and depend on many uncertain input parameters. A Gaussian process emulator based approach is proposed to simultaneously study high dimensional multivariate spatio-temporal computer model outputs for uncertainty quantification. We introduce a class of parametric covariance functions for the GP to characterize various dependence structures within and across distinct output variables, input variables, and spatio-temporal components. This flexible and interpretable class of covariance models has the advantage of modeling complex nonseparable and asymmetric dependence structures over several existing separable covariance models. Several computational strategies are investigated and compared to facilitate model implementations, including composite likelihood methods, covariance approximation methods and combinations of these methods. Finally, we apply our approach to the uncertainty quantification of ozone data.

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### MS14

### Constrained Orthogonal Decomposition for Reduced Order Modeling of High-Reynolds-number Shear Flows

We generalize the projection-based model order reduction approach by incorporating Navier-Stokes equation based constraints in the kinematic expansion. Thus, in addition to optimally represent the training data, the derived reduced order models inherent important symmetry and energy balance properties of the the Navier-Stokes equations. This approach can be used to fine-tune the dynamical system such that no stabilizing eddy-viscosity term is required - contrary to other projection-based models of high-Reynolds-number flows. The proposed method is illustrated using several test cases including twodimensional flow around a cylinder, two-dimensional flow inside a square lid-driven cavity, a two-dimensional mixing layer and three-dimensional flow around the Ahmed body. Generalizations for more Navier-Stokes constraints, e.g. Reynolds equations, can be achieved in a straightforward variation of the presented results.

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### MS14

#### Statistical Prediction of Extreme Events in Nonlinear Waves

Extreme ocean or rogue waves have attracted substantial scientific attention during the last several years because of their catastrophic impact on ships and coastal structures. To study these extreme waves, we develop a wavelet based algorithm that detects and quantifies their statistical properties in the context of the Majda-McLaughlin-Tabak (MMT) model. We show how the statistics of a critical scale allow us to predict the occurrence of these extreme waves.

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### MS14

### Sparsity, Sensitivity and Encoding/decoding of Nonlinear Dynamics using Machine Learning Methods

We show that for complex nonlinear systems, model reduction and compressive sensing strategies can be combined to great advantage for classifying, projecting, and reconstructing the relevant low-dimensional dynamics. The advocated technique provides an objective and general framework for characterizing the underlying dynamics, stability, and bifurcations of complex systems. Moreover, optimal sparse sensor placement, characterizing maximal sensitivity, can be objectively obtained.

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### $\mathbf{MS14}$

### Blended Particle Filtering Algorithms for Turbulent Dynamical Systems

We develop a blended particle filtering method for turbulent dynamical systems with high dimensional phase-spaces that possess non-Gaussian nonlinear dynamics. The state vector  $u \in \mathbb{R}^N$  of the system is decomposed into two orthogonal subspaces adaptively in time, where  $u = (u_1, u_2)$ ,  $u_i \in \mathbb{R}^{N_j}$   $(j = 1, 2, N_1 + N_2 = N)$  with the property that  $\mathbb{R}^{N_1}$  is low dimensional enough so that the statistics of  $u_1$ can be computed through a particle filtering method to capture high order statistics and the statistics of  $u_2$  are assumed to be conditional Gaussian given  $u_1$  where Kalman filter formulas can be applied. Blended uncertainty quantification algorithms (QG-DO, MQG-DO) developed by T. Sapsis and A. J. Majda are used here to calculate the two orthogonal components of the system for the forecast step. The most probable conditional Gaussian distribution in the orthogonal subspace is achieved using maximum entropy principle from information theory, yielding a simple overdetermined least square problem for particle weights after the analysis step. The filtering performances of these schemes are then assessed through a specific test model, the forty-mode Lorenz 96 system, which despite its simple formulation, presents strongly turbulent behaviour with a large number of unstable dynamical components in a variety of chaotic regimes. The blended particle filtering algorithms, with just a five dimensional dynamical filtering subspace in our test case, is able to capture the high order and non-Gaussian statistics for the L96 system, making the blended particle filtering algorithm an attractive alternative to ensemble adjustment filters as regards both filter performance and capturing non-Gaussianity in a wide range of regimes.

#### Di Qi

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### MS15

### Global Sensitivity Methods: Some Issues and Solutions

Global sensitivity analysis methods are certainly the tool we need to make the most of the output of a computer code. However, if critical aspects such as the presence of non-smootheness in the model inputs or the degree of confidence in the estimates are neglected, the information drawn by the analyst might be subotimal. In this work, we review several issues and propose possible solutions to avoid potential pitfalls.

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### MS15

### Uncertainty Quantification in the Presence of Subsurface Heterogeneity

We present deterministic CDF equations that govern the evolution of cumulative distribution function (CDF) of state variables whose dynamics are described by firstorder hyperbolic conservation laws with uncertain coefficients that parametrize the advective flux and reactive terms. The CDF equations are subject to uniquely specified boundary conditions in the phase space, thus obviating one of the major challenges encountered by more commonly used PDF (probability density function) equations. The computational burden of solving CDF equations is insensitive to the magnitude of the correlation lengths of random input parameters. This is in contrast to both Monte Carlo simulations (MCS) and direct numerical algorithms, whose computational cost increases as correlation lengths of the input parameters decrease. The CDF equations are, however, not exact since they require a closure approximation. To verify the accuracy and robustness of the LED closure, we conduct a set of numerical experiments which compared the CDFs computed with the CDF equations with those obtained via MCS. This comparison demonstrates that the CDF equations remain accurate over a wide range of statistical properties of the two input parameters, such as their correlation lengths and variance of the coefficient
that parametrizes the advective flux.

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## MS15

#### Holistic Uncertainty Management for Environmental Decision Support

Uncertainty, complexity and conflict dominate the big issues in environmental decision making. Model predictions, and resulting recommendations, might change not only depending on decisions about data, model structure and model parameters, but also formulation of a problem and how future surprises are anticipated. Based on this observation, we present a framework for identifying and managing uncertainties holistically, and then illustrate how existing techniques and processes can be integrated into this framework.

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### MS15

### On the Quantity and Quality of Information Provided by Models and Induction

A flexible interpretation of Shannons information is proposed that reconciles the intuition that models provide information with the data processing inequality, which states that models cannot add information to that contained in input data. These ideas are illustrated using some relatively simple examples in which the following are measured: the quantity and quality of information about streamflow provided by various assumptions included in a rainfallrunoff model, the process of parameter estimation, and the process of data assimilation.

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## MS16

### Uq Benchmark Problems for Multiphysics Modeling

This presentation will report on efforts coordinated with the "Committee on Uncertainty Quantification of the US-ACM' to define a set of benchmark problems relevant to uncertainty quantification of multiphysics problems. These benchmark problems will exhibit conceptual, mathematical, and computational challenges relevant to the characterization, propagation, and management of uncertainties in engineering problems that couple multiple physics.

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## MS16

## UQ Benchmark Progression of Turbulent Wall-Bounded Flows

Simulations of wall-bounded turbulent flows are of critical importance in all fields of engineering. Accurate evaluations of convective heating, aerodynamic behavior, mixing, and ultimately performance depend directly on our ability to represent turbulence close to solid boundaries. The Reynolds-averaged Navier-Stokes (RANS) equations solution for even extremely simplified configurations, such as the flow in a square duct [Bradshaw P., "Turbulent Secondary Flows", 1987], fail to predict the correct turbulence characteristics because of invalid assumptions. In this benchmark we propose to study fully-developed duct flows for a progression of duct geometries of increasing physical complexity. The objective of the benchmark is to predict, with quantified uncertainty, the velocity field in these duct for which detailed DNS results are available for comparisons. The computations, as will be demonstrated, can be performed using open-source (SU2, http://su2.stanford.edu) and commercially available software (ANSYS Fluent). A detailed description of the benchmark problem, the closure, the quantity of interest and the DNS datasets will be given at the conference.

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### MS16

### Uq Challenge Benchmarks Overview

This presentation introduces the vision and goals of the UQ Challenge Benchmarks effort. We are proposing a community approach to the challenge of developing appropriate UQ benchmarks; these benchmarks, over time, will serve as a basis for developing, assessing, and improving UQ capabilities. This is a continuation of the UQ Challenge Benchmarks minisymposium held at USNCCM12 in July, 2013.

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## $\mathbf{MS16}$

## Uq Benchmark Problems for Subsurface Flows

Not available at time of publication.

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## MS17

# Building Surrogate Models with Quantifiable Accuracy

This talk overviews a new surrogate model construction algorithm that combines generalized perturbation theory with reduced order modeling to formulate a physicsinformed surrogate model with quantifiable error bounds, meaning that one can with confidence determine the quality of the surrogate predictions, a quality that is lacking in many of the state-of-the-art surrogate techniques. A surrogate model is constructed to replace the direct solution of the neutron transport equation in nuclear reactor applications.

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#### MS17

#### Exploring High Dimensional Spaces with Hyperplane Sampling

One problem with higher dimensions is that spaces become bigger, but we still sample them with zero-dimensional points, which stays the same. One solution is k-d darts, sampling using k-dimensional hyperplanes. If we can evaluate the function along a hyperplane, substituting fixed coordinates into an equation, then great! Otherwise, we still gain efficiency by estimating the hyperplane with a surrogate, and adapting our sampling strategy using estimates of surrogate accuracy.

<u>Scott A. Mitchell</u> Sandia National Laboratories samitch@sandia.gov

## MS17

### Fourier Analysis of Stochastic Sampling Strategies for Assessing Bias and Variance in Integration

A common strategy to calculate integrals, over domains of high dimensionality, is to average estimates at stochastically sampled locations. The strategy with which the sampled locations are chosen is of utmost importance in deciding the quality of the approximation. We derive connections between the spectral properties of stochastic sampling patterns and the first and second order statistics of estimates of integration using the samples. Our equations provide insight into the assessment of stochastic sampling strategies for integration. We show that the amplitude of the expected Fourier spectrum of sampling patterns is a useful indicator of the bias when used in numerical integration. We deduce that estimator variance is directly dependent on the variance of the sampling spectrum over multiple realizations of the sampling pattern.

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#### **MS17**

# POF-Darts: Geometric Adaptive Sampling for Probability of Failure

POF-Darts estimates probability of failure using geometrically-adaptive samples. We place sample disks (hyperspheres) outside prior disks. Disk radii are equal to the estimated domain-space distance to failure. If failure and non-failure disks overlap, then the estimate was incorrect, and we adjust the radii, making more room to introduce samples near the failure threshold. Second, we estimate the volume of the union of disks. Both phases use k-d darts, hyperplane samples.

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## Rui Wang

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#### MS18

## Scalable Algorithms for Design of Experiments on Extreme Scales

Designing computational simulations to best capture uncertainty for the extreme scale requires scalable algorithms to estimate error for a broad range of situations. We will present resent work on scalable error estimation of stochastic simulations where the computations can either be guided or come from a legacy database. The focus of this talk will be to describe how these fast methods are adaptive to high performance computing.

#### Richard Archibald

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#### **MS18**

## Not available at time of publication

Not available at time of publication.

## <u>Michael Griebel</u>

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### **MS18**

## A Generalized Stochastic Collocation Approach to Constrained Optimization for Random Data Identification Problems

Characterizing stochastic model inputs to physical and engineering problems relies on approximations in highdimensional spaces, particularly in the case when the experimental data or targets are affected by large amounts of uncertainty. To approximate these high-dimensional problems we integrate a generalized adaptive sparse grid stochastic collocation method with a SPDE-constrained least squares adjoint-based parameter identification approach. Rigorously derived error estimates will be used to show the efficiency of the methods at predicting the behavior of the stochastic parameters.

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## $\mathbf{MS18}$

## Hierarchical Sparse Adaptive Sampling in High Dimension

We investigate a nested approach to building sparse, adaptive representations of response surfaces. The approach performs pseudo-spectral projections in random parameter space at each realization of the physical parameter space. This effectively allows us to adapt the global representation and tune convergence independently in both spaces. We compare the nested strategy to existing sparse adaptive approaches for simple test problems, and then examine its performance for a high-dimensional system of stiff ODEs.

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Olivier P. Le Maitre LIMSI-CNRS olm@limsi.fr

### MS19

# Bayesian Data Assimilation with Optimal Transport Maps

We present two new schemes for nonlinear filtering using optimal transport maps. First is a two-stage approach that uses optimal transportation to approximate the prior or forecast distribution; we show that it can be viewed as a nonlinear generalization of the EnKF that converges to the Bayesian posterior. Next, we present a single-stage approach that effectively performs smoothing over the interval between observations. In both cases, maps are computed efficiently through the solution of stochastic optimization problems. Numerical examples show excellent filtering performance *and* convergence to the true posterior distribution in chaotic dynamical systems (e.g., Lorenz-96) and in the filtering of rare events.

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## MS19

Reduced Stochastic Forecast Models in Data As-

#### similation

Reduced stochastic models represent an attractive framework for forecasting within data assimilation, due to their ability to represent subgrid-scale phenomena as well as their computational efficiency. In this talk we will look at how such models may be used within the context of ensemble filtering, and the advantages that they provide. In particular, we will focus on situations in which stochastic forecast models outperform deterministic ones, and ways in which stochastic models may be used to approach the important problem of model error in data assimilation. This is joint work with Georg Gottwald and Alberto Carrassi.

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## Lewis Mitchell

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#### **MS19**

#### Data Assimilation and Noise Modeling

Many applications in science and engineering require that the predictions of uncertain models be updated by information from a stream of noisy data. The model and the data jointly define a conditional probability density function (pdf), which contains all the information one has about the process of interest. A number of numerical methods can be used to find this pdf, and, given a model and data, each of these algorithms will produce a result. We are interested in the conditions under which this result is reasonable, i.e. consistent with the real-life situation one is modeling. In particular, we show that well-designed particle filters will solve those data assimilation problems that are solvable in principle.

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#### **MS19**

#### Pseudo-Orbit Data Assimilation and the Roles of Uncertainty in Multi-Model Forecasting

Pseudo-orbit Data Assimilation *PDA* illustrates a new approach to forecasting with imperfect models. The key advances are to allow long assimilation windows (unavailable to a filter), while providing information on model error as an output *ratherthanrequiringitasaninput*. PDA is used in forecast mode to make true use of multimodel dynamics via cross-pollination in time. This clarifies the meanings of uncertainty and the challenges to its quantification in real

world forecasting.

Lenny Smith London School of Economics l.smith@lse.ac.uk

## MS20

## Radiation's Role in Simulating Rare Events in Lightwave Systems

This talk investigates the role of radiation in the application of importance sampling (IS) to calculate rare event probabilities in noisy lightwave systems. Recent implementations of IS in lightwave systems combine information from low-dimensional models, derived through a perturbation approach that neglects radiation, to guide Monte Carlo simulations of high-dimensional systems. We derive a lowdimensional model that includes radiation, allowing for the construction of an IS scheme that includes radiation when simulating rare events.

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## MS20

## Models of Large Deviations and Rare Events for Optical Pulses

In optical systems, amplified spontaneous emission noise leads to errors if noise-induced fluctuations are large. We discuss methods for modeling large deviations in such systems when an optical detector is included. In particular, we show how the problem of finding large deviations can be formulated as a constrained optimization problem that combines the pulse evolution equation and a detector model. The results of the combined optimization are then used to guide importance-sampled Monte-Carlo simulations to compute error probabilities.

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#### MS20

## Assessing Uncertainty in Mode-Locked Lasers with Feedback

Mode-locked lasers used for precision time-keeping and femtosecond control of chemical reactions incorporate feedback mechanisms to control the phase difference between carrier and envelope of the electric field. In addition to increased linewidth, noise in these lasers can lead to loss of lock in the feedback mechanism, with a frequency that can be computed using finite-dimensional reductions and large deviation theory. We compare these measures of uncertainty for systems using different feedback mechanisms.

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#### MS20

#### Optimal Least Action Control for Manipulating Noisy Network Dynamics

Noise caused by small fluctuations is a fundamental part of a wide range of dynamical processes. While the response of systems to such noise has been studied extensively, there has been limited understanding of how to control this response and exploit it to lead the system to a desired state. Here we present a scalable, quantitative method based upon large deviation theory to predict and control rare noise-induced switching between different states in a dynamical process. We show how this method can be applied to a wide range of physical systems. In particular, we consider several different biological models and show how gene activation rates in genetic regulatory networks can be tuned to induce lineage changes towards pre-specified cell states, promote transdifferentiation, and predict novel multiplexing strategies for cancer therapeutics. Furthermore, the use of Wentzell-Friedlin theory for the specified noise regimes is validated through a newly developed implementation of importance sampled Monte-Carlo that is able to calculate transition rates for large, non-gradient systems. This framework offers a systems approach to identifying key factors for rationally manipulating network dynamics.

#### Danny Wells

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#### MS21

## Addressing Both Parameter and Model Form Uncertainties in Simulation-Based Robust Design

Methods have been developed in our research to systematically account for both parametric uncertainty and interpolation uncertainty, due to the lack of simulation runs, in robust design. The method uses Gaussian processes to model the costly simulator and quantify the interpolation uncertainty within a robust design objective. In this talk, sampling techniques and problem formulations will be introduced for both scenarios of uncertainty associated with design variables and that associated with noise variables.

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## **MS21**

#### Interval Model Uncertainty in Nonlinear Fea

Not available at time of publication.

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## MS21

#### Model Discrepancy in Physical System Models

Given the fallibility of models of physical systems in general, it is important to account for model discrepancy errors in the fitting of physical models to data. In this talk, I will discuss available statistical methods for accounting for model discrepancy errors, in the context of Bayesian inference. I will, more specifically, discuss issues pertaining to the application of these methods in the context of models *physical* systems in particular.

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## MS21

# Quantification of Model Form Uncertainty in Molecular Dynamics Simulation

The sources of model form uncertainty in molecular dynamics (MD) include imprecise interatomic potential functions and parameters, inaccurate boundary conditions, cutoff distance for simplification, approximations used for simulation acceleration, calibration bias caused by measurement errors, and other systematic errors during mathematical and numerical treatment. We will illustrate the sensitivity and effect of model form uncertainty in MD on property and response predictions. Generalized interval probability is used to quantify both aleatory and epistemic uncertainties.

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#### MS22

#### Calibration and Uq for Test Beds in the Ocean

Constraining full ocean models to data is challenging due to long run times for spin-up and sparse observations. Hence we consider an ocean model testbed with high-resolution models in lieu of observations. This work explores two major issues in UQ; first, qualification of parameterizations using model calibration, with structural discrepancy for model comparison. Second, we resolve information from multiple metrics using a hierarchical model accounting for correlation and strength of these information sources.

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## MS22

#### Uncertainty Quantification for NASA's Orbiting Carbon Observatory 2 Mission

NASA's Orbiting Carbon Observatory 2 (OCO-2) is scheduled for launch in July of 2014, and will provide observations of carbon dioxide concentration globally at 1 km spatial resolution. These "observations" are really inferences since satellite instruments only measure radiance spectra from which the atmospheric state is inferred. The solution to this inverse problem is implemented through a Bayesian formalism that starts with a prior on the state, and solves for the posterior distribution of the state given the radiance observations. Limits on knowledge of the physics and a multitude of practical implementation issues introduce significant uncertainties that are not accounted for by the posterior covariance matrix. In this talk, we discuss how the OCO-2 team is addressing this issue in order to provide more realistic uncertainties on the data it will provide to the science community for studying the carbon cycle.

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#### MS22

## Exploring a Cloud Microphysics Model Using Statistical Emulation

The complex and highly computational cloud model MAC3 is used to simulate the formation of deep convective clouds given a set of microphysical and atmospheric parameters, some of which are subject to a degree of uncertainty. We use a statistical emulation approach to evaluate the parametric uncertainty in this model: to identify the parameters that drive uncertainty in the model outputs from MAC3 and to quantify the cloud response to aerosol in the atmosphere.

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## MS22

### Uncertainty Quantification in Aerosol and Atmospheric Physics

Gaussian process emulation and variance-based sensitivity analyses are used to quantify temporal changes in the magnitude of contributions from uncertain aerosol parametrisations to the radiative forcing of future climate. The effect of atmospheric physics parametrisations on aerosol radiative forcing are analysed separately for a contrasting perspective of climate parametric uncertainty. Preliminary results from a simultaneous aerosol and atmospheric physics perturbed parameter ensemble reveal the relative magnitude of contributions to climate uncertainty from these sources.

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## MS23

### Model Reduction for Stochastic Fluid Flows Using Dynamically Orthogonal and Bi-Orthogonal Methods

We present two classes of time-dependent Karhunen-Loeve methods for stochastic PDEs that provide a lowdimensional representation for random fields. Both the dynamically orthogonal (DO) and bi-orthogonal (BO) have the time-dependent spatial and stochastic basis under different constraints that lead to different evolution equations. We examine the relation of the two approaches and prove theoretically and illustrate numerically their equivalence. Several examples are presented to illustrate the DO and BO methods as well as their equivalence.

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### MS23

## Mechanisms of Derivative-Based Uncertainty and Sensitivity Propagation in Barotropic Ocean Models

Not available at time of publication.

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## MS23

#### Closed-Loop Turbulence Control - A Systematic Strategy for the Nonlinearities

We propose a machine learning control strategy for arbitrary turbulent flow configurations with a finite number of actuators and sensors. This method designs and optimizes closed-loop control laws automatically detecting and exploiting linear to strongly non-linear actuation mechanisms. Presented examples range from a simple analytical mode, numerical simulations to the TUCOROM mixing layer control demonstrator. We acknowledge funding of the ANR (Chair of Excellence TUCOROM, SepaCoDe), the EC (Marie-Curie ITN) and the NSF (PIRE grant).

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## MS24

### Combining High-Dimensional Data from Climate Models and Observations to Sharpen Predictions About Future Climate

Scientists and policy makers are interested in characterizing and, if possible, reducing uncertainty about climate change projections by using observational data. When the observations are high-dimensional spatial data sets, rigorous statistical approaches for uncertainty quantification may become computationally prohibitive. We develop a computationally efficient reduced-dimensional Gaussian process-based approach that accounts for complicated error structure and data-model discrepancies. We find that using unaggregated data reduces uncertainties and results in sharper climate projections.

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## MS24

#### Spatial Temporal Uncertainty Quantification Methods for Satellite Output

Satellite data product measurements are obtained through a retrieval algorithm based on deterministic properties relating reflected radiation to the Earths physical system. NASAs Aquarius Satellite System measures sea surface salinity. Aquarius has several sources of uncertainty, with errors and bias in the salinity retrieval algorithm coming from a number of sources. We develop statistical methodology for properly quantifying uncertainties, taking into account the spatio-temporal characteristics, parameter estimation, and associated biases due to the retrieval algorithm.

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## MS24

# Influence of Climate Change on Extreme Weather Events

Not available at time of publication.

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#### MS24

#### Inference for Hidden Regular Variation in Multivariate Extremes

A fundamental deficiency of classical multivariate extreme value theory is the inability to model dependence in the presence of asymptotic independence. A framework for this is provided by hidden regular variation. We develop a representation for hidden regular variation as a sum of independent regular varying components, which is used as the basis for a likelihood-based estimation procedure employing a Monte Carlo expectation-maximization algorithm which has been modified for tail estimation. The methodology is demonstrated on simulated data and applied to air pollution measurements.

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#### MS25

Gaussian Process Adaptive Importance Sampling

#### (GPAIS)

Importance Sampling reduces Monte Carlos error by favoring important regions of input space and down-weighting those samples. The unknown ideal importance distribution yields zero error; poorly chosen importance distributions increase error. GPAIS generates sequentially improving approximations of the ideal distribution, promoting IS from a dangerous art-form to a dependable tool. Sandia National Laboratories is operated by a subsidiary of Lockheed Martin Corporation for the U.S. Department of Energys National Nuclear Security Administration under contract DE-AC04-94AL85000.

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#### MS25

#### iKriging with Big Data

The Kriging or the Gaussian process model is widely used in uncertainty quantification and statistics. From a statistical point of view, the more data you have, the better fitting you are supposed to achieve. However, the accuracy of the Kriging model may not increase with the number of points. This is because the numerical issue in inverting the covariance matrix with Big Data. To mitigate this problem, we propose a new algorithm named iKriging (a.k.a. iterative Kriging). iKriging is an iterative device. It has a desirable monotonicity property that continuously refines the accuracy of Kriging from one iteration to another. The algorithm uses a short-cut to avoid the computation of matrix inverse and is stable for Big Data. This is based on joint wok with Shifeng Xiong at Chinese Academy of Sciences.

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#### MS25

#### Compressive Sensing for Computational Materials Science Experiments

Long-standing challenges in cluster expansion (CE) construction include choosing how to truncate the expansion and which crystal structures to use for training. Compressive sensing (CS), which is emerging as a powerful tool for model construction, provides a statistical framework for addressing these challenges. A recently-developed Bayesian implementation of CS (BCS) provides a framework, a vast speed-up over current CE construction techniques, and error estimates on model coefficients. Here, we demonstrate the use of BCS to build cluster expansion models for several binary alloy systems. The speed of the method and the accuracy of the resulting fits are shown to be far superior than state-of-the-art evolutionary methods for all alloy systems shown. When combined with highthroughput first-principles frameworks, the implications of BCS are that hundreds of lattice models can be automatically constructed, paving the way to high-throughput thermodynamic modeling of alloys.

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## MS25

## Performance Modeling and Optimization in Numerical Simulations

Rapid development of computing technologies has generated unprecedented opportunities to explore complex physical phenomena via numerical simulations. However, to develop efficient simulation algorithms and codes with optimal performance remains a challenge, especially for the latest powerful yet complicated computers. Performance optimization usually involves tuning parameters arising in physical models, numerical algorithms, and computer hardware specifications. We will demonstrate how black-box computational performance can be predicted and then optimized by surrogate-assisted approaches in real applications.

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### MS26

# A Randomized Map Algorithm for Large-Scale Bayesian Inverse Problems

We present a randomized MAP algorithm for exploring the posterior of Bayesian inverse problems. The unique property of the method is the ability to generate independent samples by solving randomly perturbed MAP problems. We present the theory, practicality and application of the method on a large-scale Bayesian inverse problem governed by Helmholtz equation.

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#### MS26

Dimension-independent Likelihood-informed MCMC Samplers

Many Bayesian inference problems require exploring the

posterior distribution of high-dimensional parameters, which in principle can be described as functions. By exploiting the intrinsic low dimensionality of the likelihood function, we introduce a suite of MCMC samplers that can adapt to the local complex structure of the posterior distribution, yet are well-defined on function space. Posterior sampling in a nonlinear inverse problem and a conditioned diffusion process are used to demonstrate the efficiency of these dimension-independent likelihood-informed samplers.

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### MS26

#### Bayesian Uncertainty Quantification for Differential Equations

We develop a fully Bayesian inferential framework to quantify uncertainty in models defined by general systems of analytically intractable differential equations. This approach provides a statistical alternative to deterministic numerical integration for estimation of complex dynamic systems, and probabilistically characterises the solution uncertainty introduced when models are chaotic, ill-conditioned, or contain unmodelled functional uncertainty. Viewing solution estimation as an inference problem allows us to quantify numerical uncertainty using the tools of Bayesian function estimation, which may then be propagated through to uncertainty in the model parameters and subsequent predictions. We incorporate regularity assumptions by modelling system states in a Hilbert space with Gaussian measure, and through iterative model-based sampling we obtain a posterior measure on the space of possible solutions, rather than a single deterministic numerical solution that approximately satisfies model dynamics. We prove some useful properties of this probabilistic solution, propose efficient computational implementation, and demonstrate the methodology on a wide range of challenging forward and inverse problems. Finally, we incorporate the approach into a fully Bayesian framework for state and parameter inference from incomplete observations of the states. Our approach is successfully demonstrated on ordinary and partial differential equation models with chaotic dynamics, illconditioned mixed boundary value problems, and an example characterising parameter and state uncertainty in the Navier-Stokes equations and a biochemical signalling pathway which incorporates a nonlinear delay-feedback mechanism.

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## MS26

# Exploiting Geometry in MCMC Using Optimal Transport Theory

Non-Gaussian distributions with varying correlation structures (e.g., "banana"-shaped distributions) can dramatically reduce the efficiency of existing adaptive Markov chain Monte Carlo (MCMC) methods. Yet such distributions frequently arise as posteriors in Bayesian inference. We use transport maps to define a class of MCMC proposals that can capture important features of these densities, leading to efficient sampling. By developing a stochastic approximation update to the map, we formulate an efficient adaptive MCMC method.

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## MS27

## Stabilized Low-memory Kalman Filter for High Dimensional Data Assimilation

The Extended Kalman filter is a known algorithm used for data assimilation. However, it requires storage, multiplication and inversion of matrices that become impracticably large when state space dimension grows. This can be overcome by introducing low-memory approximations. However, the approximative covariances are not positivesemidefinite. We propose a family of stabilizing corrections which circumvent this problem. Furthermore, we demonstrate that when applied the suggested corrections imply a better convergence rate of the approximations.

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## MS27

### Filter Divergence and Enkf

The Ensemble Kalman Filter (EnKF) is a widely used tool for assimilating data with high dimensional nonlinear models. Nevertheless, our theoretical understanding of the filter is largely supported by observational evidence rather than rigorous statements. In this talk we attempt to make rigorous statements regarding "filter divergence", where the filter loses track of the underlying signal. To be specific, we focus on the more exotic phenomenon known as "catastrophic filter divergence", where the filter reaches machine infinity in finite time.

David Kelly

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## **MS27**

# Combined Parameter and State Estimation in Lagrangian Data Assimilation

Inferring parameters in a geophysical flow model is a challenge for Lagrangian data assimilation (LaDA). We present a filtering-based method that combines particle filter and ENKF to track time-varying state vectors (positions of drifters) and fixed model parameters in a quasi-geostrophic two-layer shallow water model. Our method uses a dual strategy that performs parameter estimation by particle filtering and subsequently use the "best" parameter to track the position of drifters by ENKF. This method will suit a situation where the parameter space is low-dimensional but the state vector (the drifters) is high-dimensional.

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## MS27

#### Accuracy of the Optimal Filter for Partially Observed Chaotic Dynamics

The aim of filtering is to estimate in an on-line fashion the value of a stochastic process, the signal, given some noisy observations. In this talk we study discrete time randomly initialized signals that evolve according to a deterministic map  $\Psi$ . We show conditions on  $\Psi$  which ensure that if the observations are sufficiently informative— the error made by the optimal filter when estimating the signal becomes small in the long-time asymptotic regime. Our main theorem comes as a by-product of a result, of independent interest, on the suboptimal filter known as 3dVar. As a particular example of our theory we consider chaotic signals defined via the solution, at discrete times, to a dissipative differential equation with quadratic energy-conserving nonlinearity. The Navier Stokes equations on a torus, the Lorenz 63 model and the Lorenz 96 model, observed partially and noisily, are within the scope of our analysis.

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## **MS28**

# Uncertainty Quantification in Astrophysical Simulations of White Dwarf Stars

Use of supernovae as cosmological distance indicators is limited by uncertainty in the calibrated brightness of observed explosions, and dark energy studies critically depend on controlling this uncertainty. We present a study of uncertainty in the white dwarf progenitors for these supernovae produced with the MESA stellar evolution code. We vary the composition of the protostar (an aleatory uncertainty) and a model parameter (an epistemic uncertainty) and quantify the effects on the resulting stellar evolution.

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#### MS28

#### V&V and Uncertainty Quantification for Turbulent Mixing in Inertial Confinement Fusion Capsules

We compare simulations and experiments for Inertial Confinement Fusion capsules, starting at the deceleration phase of strong Rayleigh-Taylor instability, using the software codes HYDRA, FLASH and FronTier. Improved agreement with experiment is obtained through an increase in the solution entropy, perhaps associated with uncertainties in the entropy of the capsule fuel ice layer. The extent of 2D and 3D instabilities are analyzed through a theoretical mix model and through direct simulation, also with reference to experimental observations.

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### MS28

#### Quantification of Multiple and Disparate Uncertainties in the HyShot II Scramjet

The talk will summarize the approach taken and the lessons learnt in a five-year project aimed at quantifying the effects of different types of uncertainties on the performance and the margin to failure of the HyShot II scramjet engine. Specific focus will be placed on the approach to quantify the effects of the systematic (epistemic) errors in the turbulence modeling.

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#### **MS28**

#### Uncertainty Quantification of Transient Turbulent Flows Using Dynamical Orthogonality

We employ the dynamically orthogonal field equations to perform stochastic order reduction and uncertainty quantification in fluid flows characterized by low-dimensional attractors. Using the projected dynamics we examine the geometry of the finite-dimensional attractor associated and relate its nonlinear dimensionality to energy exchanges between dynamical components of the flow. In particular, we illustrate how the shape of the attractor results from the synergistic activity of the linearly unstable and stable modes as well as the action of the quadratic terms.

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#### **MS29**

## Representing Model Form Uncertainty: A Case Study in Chemical Kinetics

We investigate model form uncertainty for a generalized problem in chemical kinetics. In a typical reaction, the complete reaction mechanism is not well-understood, necessitating an approximate model. To make predictions of given quantities of interest, a careful representation of model inadequacy must be included to account for missing dynamics. The main technique replaces deterministic differential equations with stochastic ones, driven by stochastic terms for the hidden dynamics. A central concern is to use all available information to make the best possible predictions.

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## MS29

#### Probabilistic Representations of Model Inadequacy for RANS Turbulence Models

It is well-known that RANS turbulence models fail to represent the effects of turbulence on the mean flow for many important flows. We consider probabilistic representations of this model inadequacy for wall-bounded flows. These probabilistic models are constructed based upon theoretical and empirical knowledge regarding the behavior of the Reynolds stress and the ways in which eddy-viscosity-based turbulence closures can be deficient. The resulting models are calibrated and tested using DNS data for channel flow.

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## MS29

#### Estimation of Structural Error in the Community Land Model Using Latent Heat Observations

We present the model-form error for Latent Heat as modeled by the Community Land Model (CLM). We construct a surrogate for the CLM and fit it to observations from the US-ARM and US-MOz sites to estimate 3 hydrological parameters. The formulation of the inverse problem includes a temporally correlated term to model the model-data mismatch. We compare the calibration against one where the mismatch is modeled using i.i.d. Gaussians.

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## MS30

#### Stochastic Optimization of Gas Networks

We present a stochastic optimization formulation for natural gas pipeline systems. We demonstrate that significant performance gains can be achieved over deterministic strategies.

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### MS30

#### Multilevel and Adaptive Methods for Risk-Averse PDE-Constrained Optimization

We present an adaptive, multilevel sparse-grid framework for the solution of risk-averse PDE-constrained optimization problems. Our framework uses trust-regions to manage adapted sparse-grid approximations of the objective function and gradient. This adaptivity exploits anisotropy in the stochastic space, reducing the number of sparsegrid points, while generating a hierarchy of sparse-grid discretizations. Using this hierarchy, we develop a multilevel algorithm for the approximate solution of the trust-region subproblem.

#### Drew P. Kouri

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### MS30

Topology Optimization for Nano and Macro-Scale

#### Lithography Processes with Uncertainties

The focus of this work is on incorporating manufacturing uncertainties in topology optimization of micro and nano devices. The considered fabrication process is photolithography, which transfers a mask pattern onto a substrate. The output differs from the blueprint design due to inherent limitation of the optical system and process variations. In order to obtain robust solutions, both the photolithography model and process uncertainty are included in the topology optimization process as an integrated design methodology.

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#### MS30

#### Sparse-grid Algorithms for PDE-constrained Optimization Under Uncertainty

We present an overview of algorithms for large-scale optimization of partial differential equations (PDEs) with uncertain coefficients. Our algorithms minimize risk-based objective functions using sparse-grid discretizations. We consider both unconstrained and constrained formulations, applied to examples in acoustic wave propagation and thermal fluids.

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## MS31

### Advances in Adaptive Stochastic Galerkin FEM

For PDE with stochastic data, the Adaptive Stochastic Galerkin FEM (ASGFEM) was recently introduced in [Eigel, Gittelson, Schwab, Zander, Adaptive Stochastic Galerkin FEM, accepted in CMAME] as a numerical approach which controls the error of the stochastic and the spatial discretisation simultaneously, thus in a way equilibrating these error contributions. While the initial derivation was based on the notion of the classical residual estimator, we now employ recent techniques which enable to calculate guaranteed bounds of the overall error of the discrete solution. Moreover, we extend the initial model problem to more involved settings with relevance to practical applications.

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Elmar Zander TU Braunschweig Inst. of Scientific Computing e.zander@tu-bs.de

## MS31

## Regularising Ensemble Kalman Methods for Inverse Problems

We present a novel regularizing ensemble Kalman method for solving PDE-constrained inverse problems. The proposed work combines ideas from iterative regularisation and ensemble Kalman methods to generate a derivativefree solver for inverse problems. We provide numerical results to illustrate the efficacy of the proposed method for solving Bayesian inverse problems in subsurface flow applications.

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## MS31

## Nonlinear Bayesian Updates and Low-Rank Approximations

Parameter identification is usually ill-posed. In a Bayesian setting the identification becomes a conditional expectation, and the problem is well-posed. The forward problem propagates the parameter distribution to the forecast observable. The difference leads to the update, which instead of changing the underlying measure directly updates the random variables describing the parameters by a functional approximation. The forward problem as well as the inverse problem is efficiently solved by tensor approximations.

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## MS31

## Optimal Design of Experiments: a Sparse-Integration Perspective

Both sparse, adaptive integration rules and optimization of experimental design want to explore some function with a

minimal number of function evaluations or samples. This presentation will show similarities and differences. Sparse integration could learn from experimental design in aspects of goal-oriented optimization, how to achieve robustness against noise or against improper assumptions of function classes, and how to adapt such assumptions while more function evaluation results become available.

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#### MS32

# Exploring How Parameter Importance to Prediction Changes in Parameter Space

This paper evaluates a novel, computationally frugal, hybrid local-global method for measuring how model parameter importance is distributed as parameter values change. DELSA (Distributed Evaluation of Local Sensitivity Analysis) is demonstrated using hydrologic models, and compared to Sobol and delta global sensitivity analysis methods. Insights from DELSA can be combined with field data used to identify the most relevant parts of parameter space to focus data collection and model development.

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#### MS32

### Assessment of Predictive Performance of Bayesian Model Averaging in Reactive Transport Models

Bayesian model averaging (BMA) provides an optimal way to combine the predictions of several competing models and to assess their joint predictive uncertainty. However, BMA does not always give better predictive performance than the individual models. In this study we assess the predictive performance of BMA in multiple reactive transport models and discuss the important requirements and limitations.

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#### MS32

#### Using Airborne Geophysical Data to Reduce Groundwater Model Uncertainty

We illustrate the value of airborne geophysical data for reducing uncertainty in hydrological models; an important tool for groundwater resource managers. Although geophysical data are indirectly sensitive to hydrogeological properties, they provide dense sampling of the subsurface. Electromagnetic data are simulated using typical airborne survey parameters over a synthetic hydrogeophysical test model. Geophysical parameter uncertainty is quantified using a Bayesian McMC algorithm. Uncertainty in geophysically derived hydrogeological parameters is quantified by assessing the predictive capability of the hydrological model.

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#### MS32

### A Bayesian Framework for Uncertainty Quantification with Application to Groundwater Reactive Transport Modeling

A Bayesian framework is developed to quantify predictive uncertainty caused by uncertainty in model scenarios, structures, and parameters. Variance decomposition is used to quantify relative contribution from the various sources to predictive uncertainty. The Sobol global sensitivity index is extended from parametric uncertainty to consider model and scenario uncertainty, and individual parameter sensitivity index is estimated with consideration of multiple models and scenarios. The framework is implemented using Bayesian network.

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#### MS33

## Benchmark Problems for Predictive Material Behavior, Part 1

We will describe a series of benchmark problems of increasing complexity that provide a context for demonstrating, comparing, and validating modeling, computational and algorithmic aspects of uncertainty quantification. Our focus will be on problems related to material behavior within a component or a system. The benchmark problem will aim to clarify complexity in material response, the evolution of microstructure and instabilities, and the transition from damage nucleation to failure.

#### Roger Ghanem

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### MS33

## Benchmark Problems for Predictive Material Behavior, Part 2

We will describe a series of benchmark problems of increasing complexity that provide a context for demonstrating, comparing, and validating modeling, computational and algorithmic aspects of uncertainty quantification. Our focus will be on problems related to material behavior within a component or a system. The benchmark problem will aim to clarify complexity in material response, the evolution of microstructure and instabilities, and the transition from damage nucleation to failure.

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### **MS33**

#### Validating Extrapolative Predictions: Benchmark Problems and Research Issues

To maximize the utility of computational predictions, one must validate the models underpinning those predictions. Since most predictions are necessarily extrapolations, the validation process must be applicable in this case. Here, we provide a simple model problem based on a spring-massdamper system that highlights the issues introduced by extrapolation. We discuss our approach to these issues as well as possibilities for more realistic benchmark problems. Finally, we describe further research necessary to enable reliable extrapolative predictions.

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#### **MS34**

#### A Hyperspherical Method for Discontinuity Detection

The objects studied in uncertainty quantification may inconveniently have discontinuities or be contained in an implicitly defined irregular subvolume. Standard techniques are likely to fail; even an adaptive sparse grid method may require excessive sampling to achieve a tolerance. The hypersphere approach detects and unfolds discontinuity surfaces, greatly reducing the influence of highly curved geometry, and allowing good estimates of shape and probabilistic volume.

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## $\mathbf{MS34}$

#### Sparsity in Bayesian Inversion

We consider the parametric deterministic formulation of Bayesian inverse problems with distributed parameter uncertainty. For forward problems belonging to a certain sparsity class, we quantify analytic regularity of the Bayesian posterior and prove that the parametric, deterministic density of the Bayesian posterior belongs to the same sparsity class. These results suggest in particular dimension-independent convergence rates for dataadaptive Smolyak integration algorithms. This work is supported by the European Research Council under FP7 Grant AdG247277.

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## MS34

#### Stochastic Collocation on Arbitrary Nodes via Interpolation

We present a stochastic collocation algorithm on arbitrary nodes. The method seeks to interpolate collocation data, and it allows one to correctly interpolate on any set of nodes, even those singular sets by the standard polynomial interpolation. This can be useful in high dimensional UQ, as one often can not afford the large number of simulations required by many other collocation methods. We present the mathematical framework, the least orthogonal interpolation, as well as strategies to determine optimal set of nodes. Numerical examples will be presented to demonstrate the methods.

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## MS34

### A Hierarchical, Multilevel Stochastic Collocation Method for Adaptive Acceleration of PDEs with Random Input Data

We will present an approach to adaptively accelerate a sequence of hierarchical interpolants required by a multilevel sparse grid stochastic collocation (aMLSC) method. Taking advantage of the hierarchical structure, we build new iterates and improved preconditioners, at each level, by using the interpolant from the previous level. We also provide rigorous complexity analysis of the fully discrete problem and demonstrate the increased computational efficiency, as well as bounds on the total number of iterations used by the underlying deterministic solver.

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## MS35

## Adaptive Sparse Grid Interpolation Using One-Dimensional Leja Sequences

Sparse grids are most efficient when the underlying onedimensional quadrature rules are nested. However, typically such nested rules grow exponentially with the level of the sparse grid. Leja sequences build nested nodal sets by greedily minimizing the Lebesgue constant. The resulting sequences allow the construction of multi-dimensional sparse grids that are ideal for interpolation and grow at a rate of one point per level. Convergence will be demonstrated numerically for a number of examples.

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#### MS35

#### Constructing Adaptive and Unstructured Design Samples in Multivariate Space Using Leja Sequences

Approximating parameterized functions has become a central problem in large-scale scientific computing and uncertainty quantification. Our focus is on non-intrusive surrogate construction methods that use parametric snapshots as the basis for interpolatory approximation. We discuss both adapted and non-adapted sequential constructions of parametric nodes, and illustrate the effectiveness of the approach with several examples, including comparisons against the popular sparse grid approach. We will briefly discuss extensions to adaptive approximation and hybrid Leja-sparse grid methods.

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#### MS35

### Adaptive Sampling for Bayesian Updating with Non-Intrusive Polynomial Chaos Expansions

During Bayesian updating, the probability measure changes. Thus, a polynomial chaos expansion constructed under the prior is generally not optimal under the posterior. We propose an adaptive sampling rule for nonintrusive construction of chaos expansions during sequential or iterative Bayesian updating. After each iteration or update, the chaos expansion is fitted to the current knowledge about the posterior by adding new collocation points. The new points are obtained via optimization and form nested integration rules.

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#### MS35

#### Kernel-Based Adaptive Methods in Large-Scale Cfd Problems with Uncertainties

We perform uncertainty quantification for incompressible two-phase flows. Our approach is a non-intrusive stochastic collocation method in reproducing kernel Hilbert spaces. Together with an efficient multi-GPU parallelization of the applied flow solver NaSt3DGPF and the parallel stochastic collocation tool, we achieve higher-order convergence with high performance even for large-scale UQ problems. Multi-level adaptive methods might solve error balancing, dimension-independent convergence and optimal collocation point choice. We will report on our latest results within that field.

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#### MS36

### Uncertainty Quantification in Particle Accelerators: Methods and Applications

Uncertainty Quantification (UQ) in particle accelerator science is offering a rich field for scientific activities. Access to datasets from a complex scientific object - the particle accelerator - together with results of extensive simulations can be expected. More specific, how could UQ methods improve performance measures in proton therapy? It is the hope that UQ together with appropriate multi objective optimisation techniques indeed will improve the performance of various accelerators, including therapy machines. I will introduce UQ for this new area of application and use proton therapy as the study case.

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## MS36

#### Uncertainty Quantification for Laser Driven Plasmas and Application to Astrophysical Radiative Shocks

The simulations of laser-created plasmas involve physical models whose parameters are not well known. We present the Bayesian inference method used to calibrate them and to quantify the model uncertainty. This methodology is illustrated on experiments that mimic radiative shocks observed in astrophysics. The uncertainty in the collision time of the plasma impacting an obstacle is quantified. In addition, we take the numerical uncertainty and the monotonicity of the response into account.

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## MS36

#### Uncertainty Quantification for Beam Dynamics Simulations

We use Object Oriented Parallel Accelerator Library (OPAL) to track particles in high intensity proton beam transfer line. We compare our simulations with measurements that have error bars on the evolution of the envelope and bunch length of the beam from the beginning to the end of the transfer line. The statistical convergence of the problem with illustration of the spatial distribution under mesh refinement is studied for the precise beam dynamics simulations.

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### MS36

#### Error Analysis of Lagrangian Particle Methods

Lagrangian particle methods eliminate the main difficulty of the traditional Lagrangian scheme - mesh folding in simulation of complex flows by replacing fluid cells with particles. The most known example is smooth particle hydrodynamics (SPH). We will show that SPH discretization of differential operators contains large errors and is not convergent, and outline the application domain of SPH where, despite local errors, SPH produces accurate results. Then we will present error analysis of a new Lagrangian particle method, proposed by authors, that eliminates the problems of SPH.

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### **MS37**

## Hierarchical Matrix Powered Fast Kalman Filtering and Uncertainty Quantification

Kalman filtering is frequently used in many fields for sequential data-assimilation problem. Kalman filter estimates the current state of a time evolving process based on the measurements at each time instant and the observed history of the process. The Kalman filtering has two significant steps: (i) Prediction step; (ii) Update step. When the covariance matrix is dense, both these steps are computationally expensive with a computational cost of  $\mathcal{O}(nm^2 + n^2m)$ , where *m* is the number of underlying unknowns and *n* is the number of measurements. Typically, we have  $n \ll m$ . The computational cost becomes prohibitively expensive when m is large, which is often the case in real sequential data-assimilation problems, especially in the context of geosciences. In our work, we propose an  $\mathcal{O}(n^2m)$  Kalman filter. The effectiveness of the proposed Kalman filtering algorithm is demonstrated by solving a realistic crosswell tomography problem and a synthetic problem by formulating them as a stochastic linear inverse problem. In both the above cases, the sparsity of the measurement operator can be exploited to further reduce the computational time taken though the overall complexity of the proposed Kalman filtering algorithm remains the same as  $\mathcal{O}(n^2m)$ . We perform numerical benchmarking of our algorithm by comparing it with the conventional exact Kalman filter and the ensemble Kalman filter.

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#### MS37

#### A Matern Treecode for Gaussian Process Analysis

Gaussian processes are cornerstones of statistical analysis of data with covariance structures. The covariance matrix, however, poses a major challenge for large-scale processes because of the need for computing determinants and performing inversions and other matrix operations. We have proposed several techniques for replacing these computations with matrix-vector multiplications. In this talk, we will present a treecode algorithm, together with its parallel implementation, for performing this multiplication with a matrix generated by the Matern covariance kernel. The Matern kernel is a widely used class of covariance functions for modeling spatiotemporal process with arbitrary smoothness and scales. Its use in characterizing model inadequacy has also been demonstrated in several uncertainty quantification settings.

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## MS37

## Linear-Time Factorization of Covariance Matrices

Covariance matrices are the central object in Gaussian process methods for uncertainty quantification. Common operations involving covariance matrices include applying the matrix or its inverse (inference), applying a matrix square root (sampling), or computing the log-determinant (likelihood calculations). As such, it is imperative to be able to compute with covariance matrices efficiently. In this talk, we present a fast algorithm for constructing a generalized  $LDL^*$  factorization of dense covariance matrices that facilitates each of the three tasks above. The algorithm is based on hierarchical matrix approximation and borrows heavily from fast multipole-type ideas for compressing structured linear operators. For many common covariance functions, e.g., Matérn or rational quadratic, the algorithm has essentially linear complexity.

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#### **MS37**

Uncertainty Quantification of Reservoir Performance Using Fast Reduced Order Models

Not available at time of publication.

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## MS38

#### Uncertainty Use and Needs in Space Situational Awareness

The need for an accurate covariance in Space Situation Awareness has been growing steadily the past few years. The first major use was in computing the probability of collision of objects with the ISS and Space Shuttle. Other potential uses include sensor tasking, correlating uncorrelated tracks and maneuver detection. This presentation will discuss these uses and the impact of not having a covariance that represents the actual uncertainty.

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#### **MS38**

## Uncertainty Quantification in Breakup and Uct Processing

We present the results of a numerical study on the importance of proper uncertainty quantification within a (multiple hypothesis) space surveillance tracking system. Particular attention is given to (i) the choice of coordinate system used for representing uncertainty and (ii) the choice of nonlinear filter used for propagating uncertainty. These choices not only affect orbit estimates, but also the overall tracking performance and ultimately the ability to resolve uncorrelated tracks (UCTs).

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## MS38

Coordinatization Effects on Non-Gaussian Uncer-

#### tainty for Track Initialization and Refinement

A comparison between common coordinate systems used for orbital state representation is presented for track initialization and follow-on tracking utilizing optical anglesonly measurements. A parameterized probability density function representing uniform uncertainty across all possible Earth-bound constrained orbits is constructed. This distribution is mapped into each coordinate system and a parametric Bayesian filter is applied. Performance measures of uncertainty characterization and algorithm efficiency are applied to judge the efficacy of the method in each coordinate system.

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## $\mathbf{MS38}$

# Optimal Information Collection for Space Situational Awareness

This talk will focus on recent development of mathematical and algorithmic fundamentals enable accurate characterization and propagation of uncertainty in the mathematical models for orbit propagation, data assimilation of irregularly spaced noisy data from various sources with model predictions and optimal management of available sensors to support Space Control and Space Situational Awareness (SSA). The central idea is to replace evolution of initial conditions for a dynamical system by evolution of probability density functions (pdf) for state variables. The use of the Kolmogorov equation to determine evolution of state pdf due to probabilistic uncertainty in initial or boundary conditions, model parameters and forcing function will be discussed. Furthermore, the use of information theoretic metrics will be discussed for the characterization of current state of knowledge (situational awareness) and will be used for the purpose of optimal sensor deployment.

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#### MS39

## Proposals Which Speed-Up Function Space Mcmc

Not available at time of publication.

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### MS39

A Least Squares Method for the Approximation of High Dimensional Functions Using Sparse Tensor

#### **Train Low-rank Format**

We propose a discrete least squares approach for the tensor structured approximation of multivariate functions from random (noise free) evaluations. The proposed approach relies on the use of tensor train (TT) format which is a particular tree-based hierarchical low-rank format. An approximation in this format is computed using a DMRG algorithm which results in an automatic selection of the approximation rank. Regularization methods using sparsity inducing norms and cross-validation based model selection techniques are used within the DMRG algorithm for a robust and controlled identification of high degree polynomial (or wavelet) representations of the tensor factors. Numerical results illustrate the ability of the overall methodology to detect and compute accurate low-rank approximations of high dimensional functions using only few random evaluations.

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#### MS39

### Bayesian Compressive Sensing Framework for Sparse Representations of High-Dimensional Models

Surrogate construction for high-dimensional models is challenged in two major ways: obtaining sufficient training model simulations becomes prohibitively expensive, and non-adaptive basis selection rules lead to excessively large basis sets. We enhanced select state-of-the-art tools from statistical learning to build efficient sparse surrogate representations, with quantified uncertainty, for highdimensional complex models. Specifically, Bayesian compressive sensing techniques are supplemented by iterative basis growth and weighted regularization. Application to an 80-dimensional climate land model shows promising results.

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## MS40

A Computational Method for Simulating Subsurface Flow and Reactive Transport in Heterogeneous Porous Media Embedded with Flexible Uncertainty Quantification

This talk studies a modular UQ methodology to subsurface flow and reactive transport applications in randomly heterogeneous porous media. We developed a scheme to reduce the dimension of the stochastic space. This is achieved via a doubly-nested dimension reduction by applying Karhunen-Loeve expansion to the logarithmic hydraulic conductivity field, followed by Proper Orthogonal Decomposition to the velocity field. This scheme enables the modular UQ framework to handle spatially random models efficiently while maintaining solution accuracy.

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#### MS40

#### Application of Non-Intrusive Uncertainty Quantification Methods in Multiphase Flow Simulations for Coal Gasifiers

Advanced simulation capabilities have the promise of significantly reducing the time and cost of technological process deployment for fossil fuel based clean energy solutions such as coal gasification technology. However, the credibility of the simulations needs to be established with uncertainty quantification (UQ) methods. In this study, the preliminary results in applying several UQ methodologies in multiphase flows to quantify uncertainties due to various sources in computational fluid dynamics modeling of a gasifier are presented.

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#### MS40

#### Bayesian Hierarchical Multiscale model for Calibration, Validation and Uncertainty Quantification of Subsurface Flows

Uncertainty of macro-scale transport parameters, due to the inner pore-scale structure, is studied. Realizations of random porous media are generated and a Bayesian hierarchical framework is developed to integrate pore-scale data in the macro-scale description, combining them with prior spatial information and data coming from laboratory and field scale results. Numerical upscaling and Bayesian inversion are used to calibrate effective macro-scale parameters and predictions at arbitrary spatial locations can be achieved using statistical interpolation techniques. To speed up the full Bayesian update the linear and quadratic approximations are used.

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### MS40

### A Flexible and Modular Framework for Uncertainty Quantification in Non-Linearly Coupled Multi-Physics Applications

In recent years, modularization methods have gained prominence over traditional (monolithic) problem specific strategies in the modeling and simulation of multi-physics applications. In this paper, we propose an uncertainty quantification framework for non-linearly coupled, discretetime systems with stochastic inputs and control variables. For the underlying mathematical formulation of the modular strategy, we introduce a variant of polynomial chaos expansions (PCE) known as conditional PCE as a general representation of the uncertainties propagated within each module. We describe methods of integrating intrusive and deterministic (non-intrusive) modules into a global propagation scheme, which enables flexibility in the global UQ methodology. We demonstrate and study the performance characteristics of the framework using numerical examples.

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## MS41

## Calibration of Waccm's Gravity Waves Parametrizations Using Spherical Outputs

The Whole Atmosphere Community Climate Model (WACCM) is a complex chemistry-climate model. Many parametrizations have to be set. In particular, gravity waves parametrizations can have a large impact on key variations, such as the QBO in the stratosphere. We explore the distribution of these tuning parameters. We perform an uncertainty analysis and carry out calibration by reducing the dimension of the outputs through parsimonious spherical representations.

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## MS41

# Sensitivity Analysis and Calibration a Global Aerosol Model

I will present our latest work in which we observationally constrain a global aerosol model for which we have information regarding the parameter sensitivity to the constraining variable. The sensitivity information is used to identify which parameters can be constrained in different regions and seasons and to reduce the dimensions of the problem. History matching is applied to an emulator of the aerosol model gridboxes ruling out regions of parameter space that are inconsistent with the observations.

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## MS41

## The Potential of An Observational Data Set for Calibration of a Computationally Expensive Computer Model

We measure the potential of observations to constrain a set of inputs to a computationally expensive ice sheet model. Using an emulator for computational efficiency, we find the set of inputs consistent with each member of an ensemble of model output. We argue that our ability to constrain inputs to a model using its own output as data, provides an estimate for our ability to constrain the model inputs using observations of the real system.

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### MS41

#### History Matching for the Identification and Removal of Structural Errors in Climate Models

If computer model derived forecasts, often termed "calibrated predictions", are to be anything more than worthless, great care and attention must be given to accurately quantifying model discrepancy (often termed "structural error" in climate modelling). Structural errors must be elicited from experts as they represent model deficiencies that propagate into the future. But how can this be achieved for a model as complex as a climate model? A discussion with modellers will point to a number of "known structural biases" in their model, however, it is not known whether the observed biases are really structural or if they are simply a result of errant tuning. In this talk I will present history matching, a UQ method normally used to assist in model calibration, as a method of identifying structural biases and as a formal framework for climate model tuning. We apply it to the fully coupled climate model HadCM3 (a model used in 2 IPCC reports) and show that a number of "known structural biases" present in the ocean circulation for the IPCC model are removed altogether with history matching.

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## MS42

# Reproducible Research and Uq in the SuperComputing Context

Not available at time of publication.

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### MS42

## Uq and Reliability of Computational Results

Not available at time of publication.

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### MS42

#### Relating Reproducible Research and Uq

Not available at time of publication.

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## $\mathbf{MS42}$

## An Overview of Reproducible Research, Uq, and

## V&V

Not available at time of publication.

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## MS43

#### Convergence Analysis for Multilevel Sample Variance Estimators and Application for Random Obstacle Problems

The Multilevel Monte Carlo Method (MLMC) is a recently established sampling approach for forward uncertainty propagation for problems with random parameters. In this talk we present new convergence theorems for the multilevel sample variance estimators. As a result, we prove that under certain assumptions on the parameters, the variance can be estimated at essentially the same cost as the mean, and consequently as the cost required for solution of one forward problem for a fixed deterministic set of parameters. We comment on fast and stable evaluation of the estimators suitable for parallel large scale computations. The suggested approach is applied to a class of scalar random obstacle problems, a prototype of contact between deformable bodies. In particular, we are interested in rough random obstacles modeling contact between car tires and variable road surfaces. Numerical experiments support and complete the theoretical analysis.

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#### MS43

#### Multilevel Quadrature for Elliptic Stochastic Partial Differential Equations

In this talk we show that the multilevel Monte Carlo method for elliptic stochastic partial differential equations can be interpreted as a sparse grid approximation. By using this interpretation, the method can straightforwardly be generalized to any given quadrature rule for highdimensional integrals like the quasi Monte Carlo method or Gaussian quadrature. Besides the multilevel quadrature for approximating the solutions expectation, a simple and efficient modification of the approach is proposed to compute the stochastic solutions variance. Numerical results are provided to demonstrate and quantify the approach.

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## MS43

#### **Multilevel Estimation of Rare Events**

We consider PDE-based engineering systems with uncertain inputs. Our task is the estimation of small failure probabilities associated with rare events. We employ subset simulation (Au and Beck, 2001) which reduces the computational cost by decomposition of the sample space into nested, partial failure sets. The physical discretization of the engineering system - typically done by finite elements - is fixed in each failure set. To further reduce costs we introduce a multilevel approach to subset simulation where the failure regions are computed on a hierarchy of finite element meshes. We report numerical experiments and illustrate properties of the new method.

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#### MS44

## Adaptive Basis Selection Methods for Enhancing Compressive Sensing

Not available at time of publication.

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#### MS44

#### Sensitivity Analysis in Multivariate Peridynamics Simulations with the Adaptive Sparse Grid Collocation Method

We present a non-intrusive spatially adaptive sparse grid collocation method with a piecewise polynomial hierarchical basis. The method incorporates an adaptivity criterion to reduce the number of expensive samples (simulation runs), tackle discontinuities and reach high accuracies. We simulate the impact of a high-speed projectile against a plate using peridynamics to show that our method can cope with real-world applications. The application consists of extracting sensitivity values in a forward propagation problem.

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## $\mathbf{MS44}$

## Accelerated Hierarchical Stochastic Collocation Methods for PDEs with Random Inputs

Stochastic collocation methods are commonly used to construct response surfaces for PDEs with high-dimensional random inputs. The dominant cost in the construction comes from solving the linear systems - one for each collocation point. We look to improve the performance of the linear solvers by constructing good initial vectors and preconditioners. This can be done by leveraging the hierarchical structure of the collocation construction.

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#### MS44

#### Integrated Variance as an Experimental Design Objective for Gaussian Process Regression

Gaussian process regression (GPR) and pseudospectral approximation are common approaches to creating surrogate models of complex simulations. We will discuss an integrated variance objective for experimental design with GPR, suitable for arbitrary domains and input measures. In particular, we discuss optimization approaches for minimizing the objective, and the approximation properties of the resulting point sets. We then provide a theoretical and empirical comparison of GPR with various pseudospectral approximations on several test functions and domains.

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#### MS45

#### Bayesian Inversion for Data Assimilation in Hemodynamics

Computational hemodynamics is experiencing the progressive improvement of measurement tools and numerical methods. We adopt a Bayesian approach to the inclusion of noisy velocity data in the incompressible Navier-Stokes equations. Our goal is the quantification of uncertainty affecting velocity and flow related variables of interest, all treated as random variables. We derive point estimators and we obtain confidence regions for the velocity and the wall shear stress, a flow related variable of medical relevance.

#### <u>Marta D'Elia</u>

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## $\mathbf{MS45}$

### Blood Velocity Profile Estimation Via Spatial Regression with Pde Penalization

In this work we describe a novel data assimilation technique for the estimation of blood velocity profiles, using data provided by echo-doppler. This technique, at the interface between statistics and numerical analysis, is based on the minimization of a penalized sum-of-square-error functional where the roughness penalty includes the physical knowledge on the problem under study. The proposed method provides in addition to the surface estimate also its uncertainty quantification.

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#### MS45

# Fractional-Order Viscoelasticity in One Dimensional Blood Flow Models

We employ different integer-, and for the first time, fractional-order viscoelastic models in a one-dimensional blood flow solver. Simulations are performed for a large patient-specific cranial network using four viscoelastic parameter data-sets aiming to compare different models, quantify the effect of viscoelasticity, and highlight the role played by the fractional order. Finally, we reflect the sensitivity on the input parameters by performing a detailed global sensitivity analysis study on a stochastic fractionalorder viscoelastic model.

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#### MS45

### Computational Models for Coupling 3d-1d Flow and Mass Transport Problems Applied to Shape Sensitivity Analysis and Numerical Homogenization of Vascular Networks

We develop a computational model inspired to geometrical multiscale and immersed boundary methods, aiming at solving flow and mass transport problems in a network of vessels immersed into a uniform medium. It is applied to study blood perfusion. The discretizations of the two domains are completely independent. It is prone to analyze the sensitivity of blood perfusion on the geometry of the capillary network and to apply homogenization techniques to determine macroscopic transport properties.

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## MS46

#### Compressed State Kalman Filter for Large Systems

In earth sciences, the Kalman filter (KF) allows the assimilation of data in systems with large state vectors, from the discretization of functions such as pressure, velocity, concentration, or voltage. With state dimension running in the millions, the implementation of the textbook version of KF is expensive and low-rank approximations have been devised such as EnsKF and SEEP. This presentation focuses on very large linear systems and presents a method with computational and storage cost that increase roughly linearly with the state dimension but is more accurate than EnsKF. The method is closest to SEEP but uses a fixed basis to be tailored to the characteristics of the problem, mainly the transition matrix and the system noise covariance. The error analysis that complements this study guides as to how the basis family should be selected and how many terms may be needed so that the mean and covariance of the state can be approximated with satisfactory accuracy at low cost.

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#### MS46

## Geostatistical Reduced-Order Models in Inverse Problems

Reduced-order models (ROMs) approximate the highdimensional state of a dynamic system with a lowdimensional approximation in a subspace of the state space. Properly constructed, they are used to reduce by orders of magnitude the computational cost associated with the simulation of complex dynamic systems such as flow and transport in the subsurface. However, its use in inverse modeling has been limited due to the high construction cost when the number of unknown parameter is large. In this work, we apply model reduction in inverse modeling and use the solution parameter space of under-determined and highly-parameterized geostatistical inverse problems to construct the subspace in which we seek approximate solutions for any given parameters needed in the inversion process. In geostatistical inverse modeling, the solution parameter space is spanned by the cross-covariance of measurements and parameters; hence we name the ROM as the geostatistical reduced-order model (GROM). We also show that with minor loss of accuracy in the forward model, the accuracy in parameter estimation is still high and the saving in computational cost is significant. Furthermore, the computational saving is even greater in uncertainty quantification when a number of realizations are generated with Monte Carlo simulation. This is because the GROM only needs to be constructed once for all realizations and after which we do not run the full model but the GROM that is orders of magnitude smaller.

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#### MS46

#### Fast Kalman Filter Using Hierarchical Matrices and Low-Rank Perturbative Approach

Kalman filtering is a fundamental tool in statistical time series analysis to understand the dynamics of large systems for which limited, noisy observations are available. However, standard implementations of the Kalman filter are prohibitive because they require  $\mathcal{O}(N^2)$  in memory and  $\mathcal{O}(N^3)$  in computational cost, where N is the dimension of the state variable. When the number of measurements are small, we will show how to update covariance matrices in  $\mathcal{O}(k^2N + kN \log N)$  for every time step, where  $k \ll N$  is the rank of the perturbation.

## Arvind Saibaba

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## MS46

#### Improving Computational Efficiency in Large Linear Inverse Problems: An Example from Carbon Dioxide Flux Estimation

This work proposes two approaches to lower computational costs and memory requirements for large linear inverse problems. The first algorithm can be used to multiply matrices, as long as one can be expressed as a Kronecker product of two smaller matrices. The second algorithm can be used to compute a posteriori uncertainties at aggregated spatiotemporal scales. Both algorithms have significantly lower memory requirements and computational complexity relative to direct computation of the same quantities.

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## MS47

#### High-Dimension Orbit Uncertainty Propagation Using Separated Representations

Most approximations for high-dimensional, non-Gaussian stochastic differential equations suffer from the curse of dimensionality, resulting in increased uncertainty propagation computation costs. However, the theoretical computation cost of a separated representation varies quadratically with dimension, thereby improving tractability. This presentation considers the case of an Earth-orbiting satellite and puts forward results quantifying the relationship of computation cost and dimension count using a nonintrusive algorithm to generate a separated representation for the propagation of uncertainty.

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#### MS47

## Sparse Grid Based Forward and Inverse Orbit Uncertainty Quantification

A sparse grid based orbit uncertainty quantification method is presented. The orbit uncertainty of an Earthorbiting object is represented by a six-dimensional sparse grid, which is initialized using the Smolyak rule. The sparse grid is propagated through the orbit dynamics and directly updated upon arrival of the measurement data. The orbit statistical moments are computed from the sparse grid. The method is suited for non-Gaussian orbit uncertainty and has constant computational complexity.

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### MS47

#### Collision Risk Estimation for the Magnetospheric Multiscale Mission Using Polynomial Chaos Expansions

The Magnetospheric Multiscale (MMS) Mission includes four spacecraft in formation that pose a collision risk with each other. To identify such risks and quantify the probability of collision, uncertainty propagation via polynomial chaos expansions is one of the principle tools identified for use in the mission ground system. This presentation discusses the application of polynomial chaos expansion for MMS and the methods developed to quantify the collision risk over time.

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## $\mathbf{MS47}$

# Uncertainty Propagation Using Gaussian Mixture Models

Gaussian Mixture Models (GMMs) form a compromise between the Gaussian approximation and a point cloud for Gaussian distributions that become non-Gaussian through a nonlinear transformation. A multivariate GMM is typically created by applying a univariate splitting library along a single spectral direction of the covariance matrix. We extend this concept to multivariate libraries using high dimensioned univariate libraries and a recursive formulation. The result leads to a more accurate multivariate GMM.

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#### MS48

#### A Randomized Tensor Algorithm for the Construction of Green's Functions for Elliptic sPDE's

We compute Green's functions in the canonical tensor format for a class of stochastic elliptic PDE's. A key step in the iterative algorithm is the reduction of the separation rank of intermediate approximations of a Green's function. We use randomized tensor interpolative decomposition as an alternative and/or supplement to the usual alternating least squares approach and demonstrate its performance on several examples.

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## MS48

### On the Convergence of Alternating Optimisation in Tensor Format Representations

Not available at time of publication.

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#### **MS48**

#### Dynamical Low Rank Approximation in Hierarchical Tensor Formats

We consider low rank tensor product approximation. Recently introduced hierarchical Tucker representation (e.g. Hackbusch (HT). Tyrtyshnikov et al (TT)) offer new perspectives to circumvent the curse of dimensionality, since they are only polynomially scaling with respect of the dimensions. As an improvement of the Tucker format, we will observe that, for given ranks, the hierarchical tensors form a differentiable manifold. For solving parametric PDEs arising in Uncertainty Quantification we cast this problme into an optimization problems within a prescribed tensor class. A simple optimization approach (ALS) based on alternating directions provides an efficient numerical tool, which will be demonstrated.

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## MS48

### **Rank Reduction of Parameterized Time-dependent**

## PDEs

We derive a preconditioning technique, based on a nonlinear invertible transformation of a time variable, that pushes the solution field of a parameter-dependent PDE onto a low dimensional linear manifold. This transformation then enables efficient time integration via *a priori* linear reduction methods, such as PGD, DO and DyBO. The preconditioner is found either by solving an optimization problem for rank minimization or via the solution of an adjoint ODE. Numerical demonstrations are given for the stochastic Burgers and Navier Stokes equations.

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#### **MS49**

#### Exploring Parametric Uncertainty of Weather Research and Forecasting Model

This study concerns with the quantification of parametric uncertainty of the widely used Weather Research and Forecasting (WRF) model. A list of over 20 model parameters is examined for their influence on precipitation and temperature forecasting skill over the summer seasons between 2008-2010 for the Beijing region. A global sensitivity analysis is first used to screen out the most sensitive parameters. Then a surrogate modeling based approach is used to identify their optimal parameters.

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## MS49

## Uncertainty Quantification and Risk Mitigation of CO<sub>2</sub> Leakage in Groundwater Aquifers

We developed an integrated model for simulating multiphase flow of  $CO_2$  and brine in a deep storage reservoir, through a leaky well, and subsequently multicomponent reactive transport in a shallow aquifer. Each sub-model covers its domain-specific physics. Uncertainties of conceptual models and parameters are considered together with decision variables for risk assessment of leakage-impacted aquifer volume. High-resolution and lessexpensive reduced-order models of risk profiles are approximated as polynomial functions of decision variables and uncertain parameters.

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### MS50

# Mathematical Theory for Filtering with Model Errors

Not available at time of publication.

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#### MS50

## Estimating Innovation Variance in Sequential MC from Numerical Integration Error

Particle filters for the estimation of model parameters, initial values, and non-observable component from partial, noisy observations in dynamic inverse problems may require the solution of stiff systems corresponding to particles subsequently discarded. We show that by solving the associated differential equations with numerical solvers which can handle stiffness, estimating at each time step the discretization error and using it to assign the variance of the innovation, we have a handle on stability and accuracy of the propagation and on the variance of the estimate.

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#### MS50

#### Adaptive Metropolis Algorithm Using Variational Bayesian Adaptive Kalman Filter

In this work, we propose a new adaptive Metropolis-based MCMC algorithm called the variational Bayesian adaptive Metropolis (VBAM) algorithm where the proposal covariance matrix is adapted using the variational Bayesian adaptive Kalman filter. We prove a strong law of large numbers for the VBAM algorithm. We also provide the empirical convergence results of a simulated example, where the VBAM results are compared with other existing adaptive Metropolis algorithms.

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## MS50

Sequential Statistical Inference in State-space Models Using  $\mathrm{SMC}^2$ 

Not available at time of publication.

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## MS51

## Multilevel and Weighted Reduced Basis Method for Optimal Control Problems Constrained by Stochastic PDEs

We study optimal control problems constrained by Stochastic PDEs. Well-posedness of the problem, in particular uniqueness, is proved for this problem. Moreover, we propose and analyze a multilevel and weighted reduced basis method for fast and certified solve of the problem, whose efficiency and accuracy is demonstrated by numerical experiments with stochastic dimensions ranging from 1 to 100.

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## MS51

#### A Stochastic Collocation Approach for Multi-Fidelity Model Classes

We present a novel algorithm for robustly incorporating inexpensive low-fidelity models and data into expensive highfidelity simulations. Our approach maintains high-fidelity model accuracy while requiring only low-fidelity computational effort. The method is non-intrusive and extensible, effectively working with black-box simulation tools. Our procedure can address multi-physics situations, missing parameters, and an arbitrary numbers of model with varying degrees of fidelity.

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## MS51

#### Noise Propagation and Uncertainty Quantification in Hybrid Multiphysics Models

We discuss a hybrid algorithm to couple the timedependent Ginzburg-Landau (TDGL) equation to the nearest-neighbor (NN) Ising model. This setting is a testbed for simulating multiscale systems undergoing phase transitions and nucleation. A numerical analysis of the hybrid is carried out using a surrogate TDGL hybrid derived from the original algorithm by replacing the discrete-valued Ising model with the stochastic TDGL. The latter is used to compare steady-state statistics derived from the Ising-TDGL hybrid with those calculated using a Gaussian closure of the TDGL moment hierarchy. Our results indicate that for highly nonlinear systems, such as those modeled by the TDGL, an appropriate treatment of random fluctuations at the hybrid's coupling interface is required to obtain accurate estimates of both mean and variance of the system state. Moreover, we found a good quantitative agreement between the statistics following from the Gaussian closure and the hybrid simulation results.

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### MS51

### Localized Polynomial Chaos Expansion for Differential Equations with Random Inputs

We present a localized polynomial chaos expansion for PDE with random inputs. Our method employs a domain decomposition technique to approximate the stochastic solution locally. In each subdomain, accurate approximation can be achieved and more importantly, in a random space with much reduced dimensions. An interface problem is then constructed in the original high dimensional random space to ensure an accurate global solution is obtained. The interface problem requires no PDE solver and can be solved efficiently. The major advantage of the local polynomial chaos method is that it can reduce the original high dimensional stochastic problem to a set of very low dimensional local stochastic problem, regardless the dimensionality of the original problem.

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## $\mathbf{MS52}$

# Uncertainties in Carefully Constructed Models in Epidemiology

Not available at time of publication.

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## $\mathbf{MS52}$

## Not available at time of publication

Not available at time of publication.

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## MS52

## Not available at time of publication

Not available at time of publication.

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### MS52

## Set Theoretic Approaches in Uncertainty Measures

Not available at time of publication.

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#### MS53

## The Effect of Targeted Observations with the Kalman Filter: Linear Analysis and Model Problems

We demonstrate that targeting observations with various Kalman filter data assimilation techniques can significantly reduce analysis uncertainty for both linear and nonlinear systems. First, we investigate the traditional Kalman filter for a linear model, and prove an explicit formula for the analysis uncertainty. Next, we study two nonlinear model problems, which demonstrate that the local ensemble transform Kalman filter (LETKF) with targeted observations based on largest ensemble variance is skillful in reducing analysis uncertainty.

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### $\mathbf{MS53}$

## Thinking Locally: Estimating spatially-varying parameters using LETKF

We describe a study of parameter estimation for non-global parameters using the local ensemble transform Kalman filter (LETKF). By modifying existing techniques for estimating global parameters using observational data, we present a methodology whereby spatially-varying parameters can be estimated using observations only within a localized region of space. We show that the LETKF accurately estimates parameters in two applications of this work, one involving a nonlinear chaotic conceptual model for atmospheric dynamics, and another which assimilates satellite data for sea ice extent.

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## MS53

# Assimilation of Ocean Glider Data in a 3-D Flow Model

Ocean gliders are a tool for measuring quantities of interest in the ocean such as temperature, salinity, and biological components. Unlike traditional ocean sensors–like drifters and floats–gliders use fixed wings, rudders, and buoyancy control to 'fly' through the water to desired way points, but can only determine position via GPS when surfacing. This work simulates ocean glider missions and uses data assimilation on observations of their surfacing locations to estimate the surrounding flow.

## Adam B. Mallen

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### MS53

# A Hybrid Particle-Ensemble Kalman Filter Scheme for Lagrangian Data Assimilation

Lagrangian data assimilation involves using observations of the positions of passive drifters in a flow in order to obtain a probability distribution on the underlying Eulerian flow field. Several data assimilation schemes have been studied in the context of geophysical fluid flows, but many of these have disadvantages. In this talk I will give an overview of Lagrangian data assimilation and present results from a new hybrid filter scheme applied to the shallow water equations.

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## MS54

### Active Subspace Methods in Theory and Practice

In many computational models, the outputs respond only to variations along a low-dimensional subspace of the inputs, a property often unidentified and unused. The active subspace method detects this subspace, and uses it to construct a low-dimensional surrogate model of the outputs, breaking the curse of dimensionality in many UQ problems. The efficiency and accuracy of this method is demonstrated and analyzed in UQ of geometric variability on turbomachinary performance.

## Eric Dow

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## MS54

## An Active Space Method for Exploring High Di-

#### mensional Bayesian Posterior Density

We present an active space method to form an accurate surrogate of large-scale Bayesian posterior in high dimensional parameter spaces. The method constructs a dominant subspace that is determined by the gradient of the negative log posterior at the training points. We discuss issues on how to heuristically determine a good training set, how to compute the gradient efficiently using adjoint method, etc. Results on large-scale Bayesian inversion governed by Helmhotlz equation will be presented.

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## $\mathbf{MS54}$

## Dimension Reduction in Nonlinear Statistical Inverse Problems

The Bayesian approach to inverse problems in principle requires posterior sampling in high or infinite-dimensional parameter spaces. However, the intrinsic dimensionality of such problems is affected by prior information, limited data, and the smoothing properties of the forward operator. Often only a few directions are needed to capture the change from prior to posterior. We describe a method for identifying these directions through the solution of a generalized eigenvalue problem, and extend it to nonlinear problems where the data misfit Hessian varies over parameter space. This scheme leads to more efficient Rao-Blackwellized posterior sampling schemes.

#### James R. Martin

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## $\mathbf{MS54}$

#### Subspace Adaptation in Polynomial Chaos Spaces

We present a new method for the characterization of subspaces associated with low-dimensional quantities of interest (QoI). The probability density function of these QoI is found to be concentrated around one-dimensional subspaces for which we develop projection operators. Our approach builds on the properties of Gaussian Hilbert spaces and associated tensor product spaces. The method is demonstrated on problems in multiscale modeling and elasticity.

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#### MS55

#### Real Time Optimal Experimental Design for Joint Flow and Geophysical Imaging of Dynamic Targets

We present an experimental design algorithm for a joint flow and imaging inverse problem. The joint problem allows us to solve for the initial state of a reservoir as well as the fluid velocity field, and then generate predictions. The experimental design of the imaging is determined based on training sets from these predictions. We are then able to update the covariance matrix based on realistic images of flow, and thus update the optimal design.

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#### MS55

#### Optimal Experimental Design and Model Misspecification Mitigation

Mitigation and control of uncertainty in the context of large-scale ill-posed problems is essential. While improved characterization and assimilation of prior information is key, often our ability to do so for realistic problems is rather limited. Complementary to such strives, it is instrumental to maximize the extraction of measureable information. This can be performed through improved prescription of experiments, or through improved specification of the observation model. Conventionally the latter is achieved through first principles approaches, yet, in many situations, it is possible to learn a supplement for the observation operator from the data. Such an approach may be advantageous when the modeler is agnostic to the principle sources of model-misspecification as well as when the development effort of revising the observation model explicitly is not cost effective.

#### Lior Horesh Business Analy

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## $\mathbf{MS55}$

## Bayesian Experimental Design in the Presence of Model Error

Calibration and validation of models are inherently datadriven processes. A successful calibration and validation depends on an anticipatory approach to determine the information content of data provided by future experiments. Since, the information content can only be determined with respect to available computational models, any modeling error will adversely affect model-driven data collection strategies. In this work we study the behavior of Bayesian experimental design strategies when the underlying models contain structural uncertainties.

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#### $\mathbf{MS56}$

## Selection of Polynomial Chaos Bases Via Bayesian Mixed Shrinkage Prior Model with Applications to Sparse Approximation of Pdes with Stochastic Inputs

Generalized polynomial chaos (gPC) expansions allow the representation of the solution of a stochastic system as a series of polynomial terms. In high dimensional scenarios where the measurement sampling cost is high, gPC suffer from the so called curse of dimensionality issue because the number of PC coefficients increases dramatically with the dimension of the random input variables. In that case, the evaluation of the unknown PC coefficients can be inaccurate due to over-fitting when traditional methods applied. Here, we model the PC coefficients as series of basis functions. We place the task of determination of the gPC expansion into the Bayesian model uncertainty framework and employ Bayesian Elastic Net regression modeling to evaluate it. This allows for global representation of the stochastic solution, both in random and spatial domains, avoids the over-fitting issue without any significant lose in accuracy of the gPC expansion and provides interval estimates for the PC coefficients and the solution statistics. The proposed method is suitable for, but not restricted to, problems whose stochastic solution is sparse at the stochastic level and maybe the spatial level while the deterministic solver required is expensive. Such applications can be the elliptic stochastic partial differential equations on which we demonstrate the good performance of the proposed method and compare it with others, on 1D, 14D and 40D random space.

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#### MS56

#### The Importance Sampling Technique for Understanding Rare Events in Erdos-Renyi Random Graphs

What is the probability that an Erdos-Renyi random graph has an excessive number of triangles? Conditioned on having an excessive number of triangles, what does the Erdos-Renyi random graph typically look like? When attempting to simulate the probability of these rare events, the answers to the above questions play a role in designing the importance sampling scheme. A large deviations principle is recently been discovered for rare events in Erdos-Renyi graphs; in some instances, the conditioned Erdos-Renyi random graph resembles another Erdos-Renyi random graph, whereas the more interesting case is when it exhibits a clique-like structure. In this talk, we show how we may characterize the typical behavior of the conditioned Erdos-Renyi random graph through its connection with exponential random graphs, and use the latter class of random graphs to deduce the optimal importance sampling scheme.

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#### MS56

# A Low-Order Stochastic Model for Flow Control Problem

Not available at time of publication.

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#### MS56

#### An Explicit Cross-Entropy Method for Mixture

Not available at time of publication.

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#### MS57

# Multilevel Acceleration of Stochastic Collocation Methods for SPDEs

Multilevel methods for SPDEs seek to decrease computational complexity by balancing spatial and stochastic discretization errors. Multilevel techniques have been successfully applied to Monte Carlo methods (MLMC), but can be extended to accelerate stochastic collocation (SC) approximations. In this talk, we present convergence and complexity analysis of a multilevel SC (MLSC) method, demonstrating its advantages compared to standard single-level approximations, and highlighting conditions under which a sparse grid MLSC approach is preferable to MLMC.

#### Peter Jantsch

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## MS57

## Stochastic Parameterization of Sub-Grid Latent Heat Flux for Climate Models

Stochastic parameterization enables the incorporation of sub-grid heterogeneity that is currently neglected by conventional climate parameterizations. To this effect, we incorporated a stochastic parameterization of sub-grid latent heat flux in a land-atmosphere climate model. Latent heat flux is a driver of convective precipitation, so by introducing a stochastic error term with a Dirichlet distribution, we effect the precipitation distribution. Furthermore, implementing Dirichlet boundary conditions allows us to adapt the level of incorporated variability. Simulations of these stochastically forced precipitation distributions show lengthened tails and heightened extreme event prediction. The variability factor can then be optimized with comparisons of simulated and measured atmospheric data. This method shows promise in advancing climate parameterizations that are deficient in capturing variability and perpetuate the underestimation of extremes.

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## $\mathbf{MS57}$

### Optimal Point Sets for Interpolation of Total Degree Polynomials in Moderate Dimensions

Many numerical methods in uncertainty quantification, such as stochastic collocation methods, make use of interpolation techniques. In this talk, we therefore discuss the problem of choosing good interpolation points for Lagrange interpolation of total degree polynomials on the unit cube in moderate dimensions. We compute the optimal points through a minimisation of the associated Lebesgue constant, and compare the performance of these points to other point sets frequently used in applications.

### Aretha L. Teckentrup

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#### MS57

#### Bayesian Inference for An Eddy Viscosity-Type Les Models in Simulation of Turbulent Flow Around a Cylinder

Bayesian inference is rarely applied to assess the fidelity of LES models: the large number of simulations and the long computation time per one simulation result in extremely expensive computational cost. Adaptive sparse-grid highorder stochastic collocation method is an efficient approach for Bayesian inference that greatly reduces the number of model executions. In this talk, we will discuss the performance of aSG-hSC for Bayesian inference in Smagorinsky modeling of turbulent flows past bluff bodies.

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#### **MS58**

#### Speeding Up the Evaluation of Kernel Density Estimators

One of the many difficulties in kernel density estimation is the computational complexity of evaluating the estimator in the presence of large volumes of data. In this talk we explore two possible approximations for the values of a kernel density estimator on a grid. Depending on the dimensionality of the data we consider two possible approaches — (1) the Fast Fourier Transform and the Fast Gauss Transform for one and two dimensional data; (2) and a variational approximation method for higher-dimensional data.

Zdravko Botev

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#### MS58

## A Finite Element Method for Density Estimation with Gaussian Process Priors

A variational problem characterizing the density estimator defined by the maximum a posteriori method with Gaussian process priors is derived. It is shown that this problem is well posed and can be solved with Newton's method. Numerically, the solution is approximated by a Galerkin/finite element method with piecewise multilinear functions on uniform grids. Error bounds for this method are given and numerical experiments are performed for one-, two-, and three-dimensional examples.

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## MS58

## Density Estimation with Adaptive Sparse Grids

Even though kernel density estimation is the most widely used nonparametric density estimation method, its performance highly depends on the choice of the kernel bandwidth, and it becomes computationally expensive for large data sets. Our sparse-grid-based method can overcome these drawbacks to some extent, in particular for large and moderately high-dimensional data sets. We show numerical results to demonstrate that our method is competitive with respect to accuracy and computational complexity.

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## MS58

#### **Density Estimation Trees**

Density estimation trees are the natural analog of classification and regression trees (Breiman, et al. 1984) for nonparametric multidimensional density estimation. These estimate the joint probability density function by learning a piecewise constant function structured as a decision tree. These estimators exhibit the interpretability and adaptability expected of the supervised decision trees while incurring slight loss in accuracy over more sophisticated estimators. The density estimation tree is a new tool for exploratory data analysis with unique capabilities and can also be used to sample from an estimated data distribution with just a sequence of coin-flips.

### Parikshit Ram

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## MS59

### **Distance Metrics for Chaotic Systems**

The standard way of likelihood construction is to compare data and model at given measurement instants. For chaotic dynamic systems this is not an option: practically the same model parameter and initial state values lead to different trajectories, after an initial time period of deterministic behavior. One way to 'tame' chaos is to integrate out the state variables by filtering methods. However, the filter algorithms themselves require tuning parameters, which introduce bias for model parameter estimates. Here we discuss another approach: we study the chaotic trajectories by fractal dimension concepts, and modify them to define a distance metric to compare trajectories.

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## $\mathbf{MS59}$

## Bayesian Model Calibration in the Presence of Model Discrepancy

Measurement and model errors produce uncertainty in model parameters estimated through least squares fits to data or Bayesian model calibration techniques. In many cases, model errors or discrepancies are neglected during model calibration. However, this can yield nonphysical parameter values for applications in which the effects of unmodeled dynamics are significant. It can also produce prediction intervals that are inaccurate in the sense that they do not include the correct percentage of future experimental or numerical model responses. In this presentation, we discuss techniques to quantify model discrepancy terms in a manner that yields physical parameters and correct prediction intervals. We illustrate aspects of the framework in the context of distributed structural models with highly nonlinear parameter dependencies.

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### MS59

# Experiences with Parameter Estimation in Chaotic Models

We consider techniques for estimating static parameters in chaotic models. In such cases, model simulations cannot be directly compared to observations, since errors in the initial conditions lead to large deviations from the observations. One way forward is to compare summary statistics of model simulations and observations. Alternatively, one can formulate the system as a state space model, and 'integrate out' the uncertain initial conditions using filtering methods. Here, we review our experiences with these techniques.

### Antti Solonen

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### MS59

### A Bayesian Approach to Hyperspectral Remote Sensing of Canopy LAI

Leaf area index (LAI) is one of the most important biophysical parameters of forest canopies characterizing the terrestrial ecosystem status. We develop Bayesian inversion for estimating LAI based on satellite reflectance measurements. The canopy reflectance model which forms the likelihood, includes several uncertain parameters. We model the uncertainties, and use MCMC to sample the posterior density of LAI and the nuisance parameters. This gives more reliable LAI estimates than an approach where uncertainties are ignored.

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## MS60

#### A Bayesian Approach for Global Sensitivity Analysis of Multi-Fidelity Computer Codes

Multi-fidelity computer codes are widely used in science and engineering to model physical phenomena. It is common that they have a large number of input parameters. Global sensitivity analysis aims to identify those which have the most important impact on the output. Sobol indices are a popular tool to perform such analysis. The aim of this paper is to provide a methodology to estimate the Sobol indices through a surrogate model taking into account both the estimation errors and the surrogate model errors.

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#### MS60

#### Prediction and Computer Model Calibration Using Outputs From Multiple Computer Codes

Computer simulators are frequently used to describe and explore physical processes. In some cases, several computer models, each with different or unknown degree of fidelity, are available to model the same physical system. In this work, a Bayesian predictive model for the real system is built by combining field observations and model runs from multiple computer simulators. The resulting model can be used to perform sensitivity analysis, solve inverse problems and make predictions.

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#### MS60

#### Cokriging-Based Sequential Design for Multi-Fidelity Computer Codes

Cokriging models are well suited for surrogate multi-fidelity computer codes from few simulations. In practical applications, it is common to sequentially add new simulations to obtain more accurate approximations. We propose in this paper a method of sequential design which combines both the error evaluation providing by the cokriging variance and the observed errors of a Leave-One-Out crossvalidation procedure. The main advantage of this strategy is that it not only provides the new locations where to perform simulations but also which levels of code have to be simulated.

Loic Le Gratiet

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#### **MS60**

### Addressing Multi-Fidelity Black Box Systems with Sequential Kriging Optimization Partition Envelope Method

When experimental runs are expensive or time consuming, surrogate models are often used to emulate the runs. So-called "Efficient Global Optimization" methods, also known as "Sequential Kriging Optimization" (SKO), have been found to optimize noisy stochastic black box systems effectively with minimal experimental costs. These methods have also been applied to analyze multi-fidelity black box systems, to reduce evaluation cost. Yet, one important issue for SKO methods is computational overhead. In general, the overhead to compute which experimental run to perform next is considered to be minor compared with experimental costs. However, with over 100 runs, SKO overhead can cost multiple hours and becomes an important issue. In the proposed method, the region of interest has been divided into multiple sub-regions each of which is fitted with a separate Kriging meta-model to keep overhead costs minimal. Sequential Kriging Optimization is then applied in all the sub-regions and the optimal solutions are compared. This extension is termed as Sequential Kriging Optimization Partition Envelope (SKOPE) methods. We also propose an extension of SKOPE for multi-fidelity applications. We explore all methods and the computation overhead reductions using numerical examples and examples motivated by a real world die casting gate design case study.

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### MS61

#### Bayesian Approaches to the Analysis of Computer Model Output

I discuss strategies for assessing and dealing with model error when incorporating large-scale computer model output. The discussion includes notions for incorporating multimodel ensembles. Strategies rely on hierarchical Bayesian modeling. I will review a examples with applications to ocean modeling.

Mark Berliner

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#### **MS61**

# Bayesian Prior Model Selection for Channelized Subsurface Flow Models

Nested sampling (NS) algorithm suffers from low acceptance rates when applied to channelized subsurface flow models. The efficiency of NS is improved by augmenting the training image with soft probability maps to generate new samples conforming to the likelihood constraint. This results in a significant increase of the acceptance rates and the overall algorithm efficiency. The proposed algorithm is applied for calibration and prior model selection of different channelized subsurface flow models.

#### Ahmed H. ElSheikh

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## **MS61**

#### Quantifying the Uncertainty in the Assessment of Climate Change Impact on Hydrologic Extremes using Hierarchical Bayesian Modeling

Climate change would impact the spatiotemporal variability of hydrologic extremes especially in regions with topographical variations. To quantify the uncertainty in estimating the extremes, we first develop a framework in using a spatial hierarchical Bayesian method to model the extreme runoffs based on observed runoff over the Colombia River Basin in the Pacific Northwest (PNW) USA. The generalized Pareto distribution (GPD) is employed for the analysis of extremes and the Markov Chain Monte Carlo method is employed to infer the parameters of the GPD distribution. To extend the analysis of extreme for future period (2041-2070) a distributed hydrologic model, Variable Infiltration Capacity (VIC) is driven by regional climate model (RCM) forcings and the results are compared with the historical period (1971-2000). Spatial hierarchical Bayesian model is then applied over each grid cell in the basin for both time periods and for all seasons. The estimated spatial changes in extreme runoffs over the future period vary depending on the RCM driving the hydrologic model. The hierarchical Bayesian model characterizes the spatial variations in the marginal distributions of the General Extreme Value (GEV) parameters and the corresponding 100-yr return level runoffs. Results show an increase in the 100-yr return level runoffs for most regions in particular over the high elevation areas during winter.

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## MS61

# Displacement Assimilation when Features are Essential

Traditional data assimilation is cast as amplitude data assimilation and contrasted to displacement data assimilation, the latter able to correct phase information in a physically-meaningful way. We use area-preserving maps to correct phase errors in problems wherein feature preservation is essential. An example of problem where phase information is crucial is tracking of hurricanes/cyclones/tornadoes. I will first motivate the use of this method by describing how variance minimizing techniques are less successful in problems where feature preservation/detection is critical. I will describe one of our own amplitude data assimilation methods which is capable of handling nonlinear/non-Gaussian problem, albeit of small dimension, as a benchmark of what is possible with a traditional amplitude data assimilation method. I will then contrast its results to the displacement assimilation technique and describe then how both of these approaches could be combined to obtained improved estimates of the first few moments of the posterior density of states, given observations.

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#### MS62

#### Goal-Oriented Sensitivity Analysis for lattice kinetic Monte Carlo Simulations

In this talk we propose a new class of coupling methods for the sensitivity analysis of high dimensional stochastic systems and in particular for lattice Kinetic Monte Carlo. The novelty of our construction is that the sensitivity method depends on the targeted observables, hence called goaloriented, and it is obtained as a solution of an optimization problem. Furthermore, the resulting KMC sensitivity algorithm has an easy implementation that is based on the BortzKalosLebowitz algorithms philosophy, where here events are divided in classes depending on level sets of the observable of interest. Finally, we demonstrate in several examples of diffusion-reaction lattice models that the proposed goal-oriented algorithm can be two orders of magnitude faster than existing algorithms for spatial KMC.

#### Georgios Arampatzis

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Markos A. Katsoulakis University of Massachusetts, Amherst Dept of Mathematics and Statistics markos@math.umass.edu

#### MS62

## Renyi Entropy and Robustness in Rare Event Estimation

The variational relation between relative entropy and exponential integrals can be used to formulate, in precise terms, the design of robust controls and estimates when ordinary cost criteria are used. A natural question is whether there is an analogous variational relation that is suitable when costs are determined by rare events. We discuss a variational relation in terms of Renyi entropy, and describe how it can be used to define estimators with specific robust attributes for such costs.

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#### MS62

#### Not available at time of publication

Not available at time of publication

<u>Natesh Pillai</u> Statistics Harvard pillai@fas.harvard.edu

## MS62

# Sensitivity Bounds and Error Estimates for Stochastic Models

We present an information-theoretic approach to deriving optimal, computable bounds on sensitivity indices of observables for stochastic models. The presented technique allows for deriving bounds also for path-dependent functionals. Using the rate of relative entropy the sensitivity of a wide class of observables can be bounded by Fisher information and quantities that characterize the statistics (variance, autocorrelation) of observables. The use of variational representation of relative entropy also allows for error estimation and uncertainty quantification of the coarsegrained models

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#### Petr Plechac

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## MS63

## Practical Considerations for Subspace Methods in Dakota

This talk will survey the current state of active subspace methods in Sandias Dakota software, which presently focus on input parameter space reduction. I will highlight challenges to practical implementation for general optimization, UQ, and surrogate model construction such as transformation of variable characterizations and algorithm termination criteria. Discussion addressing limiting factors will be encouraged.

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

#### MS63

## On Directional Regression for Dimension Reduction

We introduce a general theory for nonlinear sufficient dimension reduction, and explore its ramifications and scope. This theory subsumes recent work employing reproducing kernel Hilbert spaces, and reveals many parallels between linear and nonlinear sufficient dimension reduction. Using these parallels we analyze the properties of existing methods and develop new ones. We compare our estimators with existing methods by simulation and on actual data sets.

Bing Li Department of Statistics Penn State bing@stat.psu.edu

#### **MS63**

Active Subspace Identification in Surrogate Mod-

## eling

Discovering the active subspace of a function enables surrogate modeling to be carried out in that low-dimensional subspace, reducing the computational burden in function evaluations to obtain training data. In this case, Experiment design, normally performed over a hypercube, is sought to be performed over a polyhedron. In this talk we review active subspace identification, and several optimization approaches for experiment design. We illustrate the methodology on several examples drawn from gas-phase combustion chemistry.

#### Andrew Packard

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#### MS63

### Family-Direction-Selective Technique for Adaptive Multidimensional Hierarchical Sparse Grid Sampling

We propose an adaptive hierarchical multidimensional sampling technique with direction and family selectivity for interpolation of a complex multiphysics models. We apply the approach to the problem of combustion engine stability and understanding the nature of cycle-to-cycle variations in power output. We take a computationally expensive engine model and replace it by a cheap interpolant to study the correlation between the various operation parameters and the engine stability.

Miroslav Stoyanov Oak Ridge National Lab mkstoyanov@gmail.com

#### **MS64**

#### Optimal Information Trajectory Design for Dynamic State Estimation

This research describes a robust methodology for optimal sensor deployment while taking into account the uncertainties in the system dynamics and measurement model. Information theoretic metrics will be developed for the characterization of current state of knowledge (situational awareness) and will be used for the purpose of optimal sensor deployment. This is a computationally expensive problem and at times intractable. In this work, an iterative sub-optimal control approach is proposed with the intent of a real-time application. Proposed methodology has wide applications in target tracking, meteorology, plume tracking and source localization.

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#### MS64

# Sequential Experimental Design Using Dynamic Programming and Optimal Maps

How can one select a *sequence* of experiments to maximize the value of costly experimental data? We formulate this optimal sequential experimental design problem by maximizing the expected information gain under continuous parameter, design, and observation spaces using a dynamic programming structure. We solve the problem numerically by (1) using optimal maps to represent posterior distributions in a sequential Bayesian inference context, and (2) using approximate dynamic programming strategies to find the optimal policy. Results are demonstrated on nonlinear/non-Gaussian inference problems.

## Xun Huan, Youssef M. Marzouk

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## MS64

## Rapid Data Gathering using Mobile Robotic Vehicles

We consider the problem of data gathering using mobile vehicles, for example by picturing target locations. We are particularly concerned with the design of the datagathering vehicles. To achieve good performance, how good perception capabilities (for recognizing targets) do they require? How agile should they be? Do they really need on board computing power to analyze the pictures that they collect on the fly, or can this analysis be left to a base station?

<u>Sertac Karaman</u> Massachusetts Institute of Technology sertac@mit.edu

### MS64

## A Framework for Sequential Experimental Design for Inverse Problems

Tikhonov regularization is to obtain regularized solutions of ill-posed linear inverse problems. We use its natural connection to optimal Bayes estimators to determine optimal experimental designs for regularizes ill-posed problems. They are designed to control a measure of total relative efficiency. We present an iterative/semidefinite programming method to explore the configuration space efficiently. Two examples from geophysics are used to illustrate the methodology.

<u>Luis Tenorio</u> Colorado School of Mines ltenorio@mines.edu

#### MS65

#### A Robust Approach to Computing Sensitivity to Serial Dependency in Input Processes

We propose a new non-parametric sensitivity analysis framework for stochastic systems that arise in operations research applications. The methodology is based on infinitesimal analysis of suitably posted optimization programs that capture the worst and best-case deviations of performance measures over the model space. This framework is completely parameter-free, computationally tractable, and can be flexibly adapted to handle specific statistical features, such as serial dependency and moment conditions, of the input model by placing appropriate constraints.

## Henry Lam

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#### MS65

#### Simulating Rare Events in Groundwater Contaminant Transport

The processes of groundwater contaminant transport are subject to various types of uncertainty. In particular, the hydraulic conductivity is often unavailable and characterized as a spatial random field. Here we present a method to simulate rare yet important events in the contaminant transport processes driven by such random field coefficients.

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#### MS65

# Hybrid Parallel Minimum Action Method and Its Applications

In this work, we report a hybrid (MPI/OpenMP) parallelization strategy for the minimum action method. For nonlinear dynamical systems, the minimum action method is a useful numerical tool to study the transition behavior induced by small noise and the structure of the phase space. To enhance the efficiency of the minimum action method for general dynamical systems we consider parallel computing. In particular, we present a hybrid parallelization strategy based on MPI and OpenMP. The application to Navier-Stokes equations will be discussed.

## Xiaoliang Wan

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#### MS65

#### Large Deviations and Importance Sampling for Anomalous Shock Displacement

In this presentation, we use a large-deviation-based importance sampling technique to efficiently compute the small probability of the event that a wave has anomalous displacements due to random forcing. In addition, we use the same technique to compute he small probability of the unstart of a hypersonic engine because of shock waves with random perturbations.

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## MS66

#### Sensitivity Analysis and Uncertainty in Groundwater Flow

Sensitivity analysis and uncertainty quantification have long been considered complementary. In systems with spatially varying parameters, the Fréchet derivative provides a local measure of system sensitivity. We show how the spectral decomposition of the Fréchet operator leads naturally to a hierarchical ordering of local variations to which the the model output is most sensitive and use these to form families of physically meaningful reduced order models that can be used in uncertainty propagation as well as parameter estimation

#### Vitor Nunes

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#### MS66

## Multilevel Sparse Grid Methods for Pdes with Random Parameters

Multilevel Monte Carlo methods improve upon the efficiency of traditional sampling schemes through the use of a hierarchy of spatial discretization models. We show how these algorithms can be extended to stochastic collocation schemes, how quadrature nesting can be exploited without compromising parallelizability, how efficiencies brought about by iterative solvers can be incorporated, and how multilevel convergence can be used to inform adaptive spatial refinement strategies.

Hans-Werner Van Wyk Department of Scientific Computing The Florida State University hvanwyk@fsu.edu

## $\mathbf{MS67}$

### Sequential Design with Mutual Information for Computer Experiments (MICE). Emulation of a Tsunami Simulator

Computer experiments are often used as substitutes for real-life experiments that are too costly, or difficult to perform. However, high-fidelity computer experiments are often highly complex and time-consuming to run. We will present a sequential algorithm based on the mutual information criterion for constructing efficient emulators for such computer experiments. The Gaussian process emulator is used, which provides explicit measure of the uncertainty in the prediction. The algorithm is demonstrated for a tsunami computer simulator.

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#### MS67

#### Data-Driven Model Reduction for the Bayesian Solution of Inverse Problems

A novel data-driven model reduction technique is developed for solving large-scale inverse problems. The proposed technique exploits the fact that the solution of the inverse problem often concentrates on a low dimensional manifold. Unlike typical MCMC approaches for solving the inverse problem, our approach avoids repeated evaluation of expensive forward models by coupling the inference algorithm with the reduced-order model. This maintains the accuracy of the inference and also results in a lowerdimensional reduced model than obtained with the typical POD approach.

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#### **MS67**

## Approximate Marginalization of Source and Detector Coupling and Location Errors in Diffuse Optical Tomography

In the Bayesian inversion framework, all unknowns are treated as random variables and all uncertainties can be modeled systematically. Recently, the approximation error approach has been 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 application of the approximation error approach for approximate marginalization of model errors caused by inaccurately known source and detector coupling and location parameters in diffuse optical tomography.

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## <u>Ville P. Kolehmainen</u>

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### MS67

## Ensemble Real-Time Control: Uncertainty, Data, Decisions.

Ensemble real-time control provides robust strategies that acknowledge uncertainties in a system's response but require many predictive simulations. Predictions derived from reduced-order models are less computationally demanding than full-order predictions but may also be less accurate. Sequential measurement updating makes reduced order approximations more attractive by continually correcting imperfect predictions. This talk uses examples to show how ensemble control with model reduction and sequential estimation can provide robust strategies that deal fox@physics.otago.ac.nz with uncertainty.

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#### **MS68**

#### Inference with Continuous-Time Markov Jump Processes Via the Van Kampen Expansion

In this talk we discuss how to use asymptotic analysis to derive a surrogate model aimed at approximating the likelihood function of partially observed phenomena that can be modeled as a continuous-time Markov jump process. Worked examples will be offered to discuss the validity and shortcomings of this approach.

Marcos A. Capistran CIMAT Mexico marcos@cimat.mx

## **MS68**

#### Estimating Baye's Factors of Approximate Numerical and Theoretical Posteriors for Optimal Precision Evaluation in the Bayesian Analysis of ODEs

To compare numerical and theoretical posteriors we propose using Bayes' Factors (BF). We prove that the BF of the theoretical vs the numerical posterior tends to one in the same order as the order of the numerical forward map solver. The BF may be already nearly one for step sizes that would take far less computational effort. A big CPU time may be saved by using coarser solvers that nevertheless produce practically error less posteriors.

J. Andrés Christen CIMAT, Mexico jac@cimat.mx

### **MS68**

#### Matrix Splittings As Generalized Langevin and Hamiltonian Proposals for MCMC

We investigate the relationship between Langevin and Hamiltonian proposals for Metropolis-Hastings methods applied to Gaussian target distributions. We find these sampling methods correspond to matrix splittings used to derive stationary linear iterative solvers, i.e. generate AR(1) processes. This correspondence helps explain the poor performance, and how to choose more efficient proposals.

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Colin Fox University of Otago, New Zealand

#### **MS68**

#### Using Polynomials to Sample from Large Gaussians Used to Model 3-D Confocal Microscope Images of **Biofilms**

Multivariate Gaussians and systems of linear equations are both specified by a quadratic form. This similarity can be exploited to produce samples from Gaussians using well established iterative techniques from numerical linear algebra. This talk will make clear how to apply Chebyshev polynomials to Gibbs samplers to speed up the geometric convergence of this class of samplers. This sampler is applied to quantify the uncertainty of biofilm volumes estimated from videos of 3-D confocol microscope images after application of anti-microbial treatments.

## Albert Parker

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#### **MS69**

## Numerical Analysis of the Advection-Diffusion of a Solute in Porous Media with Uncertainty

We consider a probabilistic numerical method to compute the spread, and its derivative the macro-dispersion, of a solute in a porous medium in the presence of uncertainty. A Monte-Carlo method is used to deal with uncertainty, and the solution of the advection-diffusion equation is approximated thanks to the time discretization of SDEs. Error estimates are established, under some assumptions including the case of random fields of lognormal type with low regularity.

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### **MS69**

#### Computation of Macro Spreading in 3D Porous Media with Uncertain Data

We consider an heterogeneous porous media where the conductivity is described by probability laws. Thus the velocity, which is solution of the flow equation, is also a random field, taken as input in the transport equation of a solute. The objective is to get statistics about the spreading and the macro dispersion of the solute. We use a mixed finite element method to compute the velocity and a lagrangian method to compute the spreading. Uncertainty is dealt with a classical Monte-Carlo method, which is well-suited for high heterogeneities and small correlation lengths. We give an explicit formulation of the macro dispersion and a priori error estimates. Numerical experiments with large 3D domains are done with the software PARADIS of the platform H2OLab.

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#### MS69

#### Stochastic Collocation for Elliptic Pdes with Random Data - The Lognormal Case

We investigate the stochastic collocation method for parametric elliptic partial differential equations (PDEs) with lognormally distributed random parameters in mixed formulation. Such problems arise, e.g., in uncertainty quantification studies for flow in porous media with random conductivity. We show the analytic dependence of the solution of the PDE w.r.t. the parameters and use this to show convergence of the sparse grid stochastic collocation method. This work fills some remaining theoretical gaps for the application of stochastic collocation in case of elliptic PDEs where the diffusion coefficient is not strictly bounded away from zero w.r.t. the parameters. We illustrate our results for a simple groundwater flow problem.

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#### MS69

#### Multilevel Monte Carlo Methods for Uncertainty Quantification in Subsurface Flow

To overcome the problem of the prohibitively large computational cost of standard Monte Carlo simulations in subsurface flow computations, we employ a new multilevel Monte Carlo algorithm, based on a hierarchy of spatial levels/grids. We provide a full convergence analysis of the multilevel algorithm in the case of a log-normal model of the rock permeability, which is frequently used in applications.

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#### MS70

#### Not available at time of publication

Zakai equations are stochastic parabolic PDEs whose solutions are the conditional probability density functions of nonlinear filter problems. There have been numerous attempts to solve nonlinear filter problems through numerical solutions of the Zakai equation. There are three obstacles in the construction of efficient numerical algorithms for the Zakai equation: 1) unbounded domain; 2) high dimensionality; 3) low regularity. In this talk, we present an efficient numerical algorithm using adaptive sampling technique to solve the equation on a time dependent bounded domain. On this bounded domain we use the sparse grid technique to reduce the complexity when solving the Zakai equation with a split up finite difference scheme.

Yanzhao Cao

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#### **MS70**

### Active Subspace Sensitivity Analysis for Fully Coupled Systems with Independent Parameters

As multiphysics models grow in complexity, the need for useful and consistent strength-of-coupling metrics increases. Such metrics are well-developed in linear models, but their applicability is limited in nonlinear models due to their local nature. I propose a new set of global metrics for strength-of-coupling based on ensemble averages of local sensitivity-based metrics. These metrics will provide insights into the physical systems, enable comparison of coupling strategies, and reveal methods for accelerating the solution procedure.

Paul Constantine Colorado School of Mines Applied Mathematics and Statistics pconstan@mines.edu

#### MS70

#### A Domain Decomposition Approach for Uncertainty Analysis

This talk proposes a decomposition approach for uncertainty analysis of systems governed by partial differential equations (PDEs). The system is split into local components using domain decomposition. Our domaindecomposed uncertainty quantification (DDUQ) approach performs uncertainty analysis independently on each local component in an "offline" phase, and then assembles global uncertainty analysis results using pre-computed local information in an "online" phase. At the heart of the DDUQ approach is importance sampling, which weights the pre-computed local PDE solutions appropriately so as to satisfy the domain decomposition coupling conditions. To avoid global PDE solves in the online phase, a proper orthogonal decomposition reduced model provides an efficient approximate representation of the coupling functions.

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#### $\mathbf{MS70}$

#### Multi-resolution Method for Emulator Construction

We introduce a multi-resolution scheme for an emulator construction on a high-dimensional parameter space. The proposed scheme overcomes some limitations of the parameter selection in the construction of Bayesian emulators, which always involves repeated inversion of a error "correlation matrix", R. The requirement of matrix inversion restricts emulators to small amounts of data mostly because for "large" N: 1) R is poorly conditioned and 2) cost of inverting matrix is  $\mathcal{O}(N^3)$  operations. Our scheme is based on mutual distances between data points and on a continuous extension of Gaussian functions. It uses a coarse-to-fine hierarchy of the multi-resolution decomposition of a Gaussian kernel.

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#### MS71

### Mitigating Observation Error Undersamling in the Stochastic EnKF

The stochastic ensemble Kalman filter (EnKF) updates its ensemble members with observations perturbed by noise that are sampled from the distribution of the observation errors. This might however introduce noise into the system, particularly when the ensemble size is smaller then the rank of the observational error covariance matrix, which is often the case in real oceanic and atmospheric data assimilation applications. This contribution presents an efficient scheme to mitigate the impact of observational error undersampling in the analysis step of the EnKF, which should provide a more accurate analysis error covariance matrices. The new scheme is simple to implement within the EnKF framework, only requiring the computation of a r-1 rank matrix approximation of the rank r EnKF forecast error covariance matrix. I will describe the new scheme and show results from numerical experiments comparing performances with standard square-root EnKFs.

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#### MS71

#### Bayesian History Matching and Uncertainty Quantification under Sparse Priors: A Randomized Maximum Likelihood Approach

Not available at time of publication.

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#### MS71

### Pragmatic Aspects of Quadrature for Propagating Uncertainty

When uncertainty is propagated with the aid of polynomial expansions. the probability density of uncertain inputs determines the set of orthogonal polynomials, and the coefficients of the expansions can be determined by quadrature. Inputs corresponding to the quadrature points are propagated, and the polynomials interpolate the resulting outputs so that outputs can be estimated for arbitrary inputs. As propagating inputs can be expensive, choice of quadrature points deserves attention. For example, are all quadrature points reasonable values for inputs? For classical methods, such as Gauss-Hermite quadrature, which provide uniform accuracy for the entire infinite range of the inputs, quadrature points extend far into the tails of the density, even to the extent that their propagation might become problematic and corresponding outputs are not representative. This suggests choosing quadrature points so that greatest accuracy is sought in a specified region of interest.

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#### MS71

### A Diagnostic Approach to Model Evaluation: Approximate Bayesian Computation

The ever increasing pace of computational power, along with continued advances in measurement technologies and improvements in process understanding has stimulated the development of increasingly complex numerical models. Reconciling these high-order system models with perpetually larger volumes of field data is becoming increasingly difficult, particularly because classical statistical methods lack the power to detect and pinpoint deficiencies in the model structure. In this talk, I will introduce a more robust and powerful method of model evaluation.

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#### MS72

### Geometric Methods for the Approximation of High-dimensional Dynamical Systems

We discuss techniques for studying, in a quantitative fashion, certain properties of high-dimensional dynamical systems in view of performing model reduction, while preserving short and large time properties of the system. In particular, in the context of molecular dynamics we will discuss techniques for estimating, in a robust fashion, an effective number of degrees of freedom of the system, which may vary in the state space of the system, and a local scale where the dynamics is well-approximated by a reduced dynamics with a small number of degrees of freedom. We use these ideas in two ways: (1) given long trajectories of the system, to produce an approximation to the propagator of the system and obtain reaction coordinates for the system that capture the large time behavior of the dynamics; (2) to learn, given local short parallel simulations, a family of local approximations to the system, that can be pieced together to form a fast global reduced model for the system, for which we can guarantee (under suitable assumptions) that large time accuracy is bounded by the small time accuracy of the local simulators. We discuss applications to homogenization of rough diffusions in low and high dimensions, as well as to molecular dynamics.

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#### MS72

#### Modelling and Estimating Multivariate Jump Diffusion Models

We develop a hierarchical model for detecting jumps in multivariate diffusion models. We construct carefully the prior for detecting jumps in individual series and proceed to define a model for dependent jumps across different series. We develop the MCMC methodology required for estimating such models from data. We illustrate the approach on financial data.

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#### MS72

# PDF Method for Langevin Dynamics Driven by Colored Noise

Not available at time of publication.

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#### MS72

### Stratification of Markov Processes for Rare Event Simulation

I will discuss an ensemble sampling scheme based on a decomposition of the target average of interest into subproblems that are each individually easier to solve and can be solved in parallel. An extension of the Nonequilibrium Umbrella Sampling Scheme of Dinner and coworkers, the scheme is capable of computing very general averages with respect to an underlying Markov process and offers a natural way to parallelize in both time and space.

#### Jonathan Weare

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#### MS73

#### A Primal-Dual Algorithm for Backward Stochastic Differential Equations

We generalize the primal-dual methodology, which is popular in the pricing of early-exercise options, to a backward dynamic programming equation associated with time discretization schemes of BSDEs. Taking as an input some approximate solution, which was pre-computed, e.g., by leastsquares Monte Carlo, our methodology allows to construct a confidence interval for the unknown true solution of the time discretized BSDE. We numerically demonstrate the practical applicability of our method in five-dimensional nonlinear pricing problems.

#### Christian Bender

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#### MS73

#### Efficient Empirical Regression Methods for Solving Forward-Backward Stochastic Differential Equations

We will present recent convergence results about the resolution of BSDEs and FBSDEs using empirical regression schemes: we will address the quadratic case, the highdimensional setting, under data with low regularity. Using Multi-Step forward dynamic programming Equations, we will show how convergence rates are theoretically improved, compared to the usual One-Step DPE; in addition, the use of DPE with Malliavin weights allows better estimates of the Z component (the gradient).

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#### MS73

#### A Fundamental Convergence Theorem of Numerical Methods for BSDEs

In this talk we review fundamental convergence theorems of numerical methods for SDEs, SDDEs and NSDDEs, and we present a new fundamental convergence theorem of numerical methods for BSDEs.

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#### MS73

#### A New Kind of Multistep Method for Forward Backward Stochastic Differential Equations

In this talk we will introduce a new kind of multistep numerical method for solving forward-backward stochastic differential equations. This method is easy to be used. Numerical tests show that the method is stable, and high accurate.

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#### MS74

#### Cross Validation for Uncertainty Quantification Using Sparse Grids

We present novel approaches for UQ parameter estimation. Specifically, we incorporate slicing and cross validation into a sparse grids framework for numerical integration. From the setting of sparse grid-based numerical integration, we slice the sparse grid and examine, for each slice, numerical integral estimates. We then apply k-fold cross validation to predict variance of numerical integral estimates. We also present related cross validation methods for numerical integration with Latin hypercube types of designs.

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#### MS74

#### **Two-Stage Predictor Design in High Dimensions**

A two-stage strategy is introduced in the context of high dimensional data (large p, small n). This arises in designing a multi-sample experiment for developing a predictor of future response, e.g., a disease state, based on a set of high dimensional measurements, e.g., a molecular assay like a gene expression microarray. The first stage of the two-stage predictor uses Predictive Correlation Screening (PCS) to select a subset of predictor variables that are important for prediction. Selected variables are used in the second stage to learn an optimal predictor. Under sampling budget constraints we derive the optimal sample allocation rules for sample sizing and variable sizing the first and second stages of the two-stage predictor. Superiority of the proposed two-stage predictor relative to competing methods, including correlation learning and LASSO, will be shown in the context of predicting health and disease. This is a collaboration with Hamed Firouzi and Bala Rajaratnam

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#### Alfred O. Hero

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#### **MS74**

#### Bayesian Subgroup Finding by Stochastic Optimization

We use inhomogeneous Markov chain simulation to solve a subgroup analysis problem. Subgroup analysis refers to the report of exceptions to the overall conclusion in a clinical trial. The large number of possible subgroups that could be reported gives rise to massive multiplicity concerns. We use a model-based and decision theoretic approach to address the problem. The proposed approach extends classical Bayesian experimental design methods in multiple ways. First, we use a carefully considered problem-specific utility function instead of commonly used default inference loss. Second, we use simulation based methods to find optimal and near-optimal designs. We use a variation of Markov chain Monte Carlo methods that are extensively used for posterior simulation to solve the optimization of posterior expected utility in the decision problem. Finally, the use of coherent posterior probabilities and the calibration of tuning parameters by (frequentist) operating characteristics can be argued to address the massive multiplicity problem that is inherent in the subgroup analysis.

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#### MS75

#### Analysis of the Lennard-Jones-38 Stochastic Network at Temperatures from Zero to the Melting Point

The Lennard-Jones-38 (LJ38) network created by Waless group exemplifies a large stochastic network with detailed balance and temperature-dependent pairwise transition rates. I will discuss the asymptotic zero-temperature pathway between the two lowest minima and its range of validity, an effective description of the transition process beyond this range, and the temperature-dependence of the transition rate between the two lowest minima.

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#### MS75

# Rare Event Simulation for Reflecting Brownian Motion via Splitting Algorithm

In this work we discuss the development of efficient splitting algorithm for estimating rare event probabilities in reflected brownian motion (RBM). In particular we are interested in the probability of the system reaching a large level before returning to a recurrent set. Splitting algorithms are defined by the level sets of so called 'Importance Functions'. Following the approach of Dean and Dupuis (2009) we based the construction of our Importance Function on subsolutions to variational problems associated with the rare event of interest.

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#### MS75

### Sampling Saddle Point on the Free Energy Surface of Complex Systems

I will present a method for finding the saddle points on the free energy surface "on-the-fly' without having to find the free energy function itself. This is done using the general strategy of the heterogeneous multi-scale method, by applying a macro-scale solver, here the gentlest ascent dynamics algorithm, with the needed force and Hessian values computed on-the-fly using a micro-scale model such as molecular dynamics. The algorithm is capable of dealing with problems involving many coarse-grained variables. The utility of the algorithm is illustrated by studying the saddle points associated with (a) the isomerization transition of the alanine dipeptide using two coarse-grained variables, specifically the Ramachandran dihedral angles, (b) the beta-hairpin structure of the alanine decamer using twenty coarse-grained variables, specifically the full set of Ramachandran angle pairs associated with each residue.

Amit Samanta

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#### MS75

#### Quantification of Extremely High Excursion Solution of Elliptic Equation with Random Coefficients

We study the high excursion behavior of the solution to a linear elliptic PDE with random coefficients. This problem is motivated by the failure problem for brittle material in which the extremely large value of the displacement or the strain or the stress field is related to the breakdown of a bulk brittle material. The Gaussian random function is applied to model the uncertainty of the elasticity parameter. We demonstrate an efficient importance sampling scheme to calculate the probability of such extreme behaviors, or the failure probability. This is joint work with Jingchen Liu and Jianfeng Lu.

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#### MS76

#### Sequential Strategies Based on Bayesian Uncertainty Quantification for Linear Sparse Surrogate Models

To quantify the uncertainty of linear sparse surrogate models, a Bayesian approach is used by imposing normal priors on the large space of coefficients. Then uncertainty quantification of surrogate models is inferred from the samples of the posterior distributions of prediction values. Unlike Kriging-based sequential procedures, our sequential strategies are designed only based on posterior samples. Three different sequential strategies are illustrated based on the different scenarios, for example, optimization and surrogate fitting.

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#### MS76

#### **Connecting Model-Based Predictions to Reality**

Not available at time of publication

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#### MS76

#### A Multiple-Response Approach to Improving Identifiability in Model Calibration and Bias Correction

Previous research has shown that identifiability in model calibration and bias correction can be improved by experimentally measuring multiple responses of the system that share a mutual dependence on a common set of calibration parameters. In this talk, we will present how to select the most appropriate subset of responses to measure experimentally using a preposterior analysis approach to predict the degree of identifiability before conducting physical experiments.

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#### MS76

#### A Theoretical Framework for Calibration in Computer Models: Parametrization, Estimation and Convergence Properties

Calibration parameters in deterministic computer experiments are those attributes that cannot be measured or available in physical experiments. Kennedy and OHagan (2001) suggested an approach to estimate them by using data from physical experiments and computer simulations. A theoretical framework is given which allows us to study the issues of parameter identifiability and estimation. It is shown that a simplified version of the original KO method leads to asymptotically inconsistent calibration. This calibration inconsistency can be remedied by modifying the original estimation procedure. A novel calibration method, called the L2 calibration, is proposed and proven to be consistent and enjoys optimal convergence rate. A numerical example and some mathematical analysis are used to illustrate the source of the inconsistency problem. (based on joint work with Dr. Rui Tuo of Chinese Academy of Sciences.)

#### Jeff Wu

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#### **MS77**

#### A Local Approximation Framework for Accelerating MCMC with Computationally Intensive Models

The application of Bayesian inference via Markov chain Monte Carlo is often limited by the expense of repeatedly evaluating the forward model. Previous work has explored global approximations of the forward model, thereby decoupling MCMC iterations from evaluation of the model altogether. These techniques provide significant empirical performance improvements, but sample from an approximate distribution. We present a new approach for incrementally constructing local quadratic approximations during MCMC, which provably yields convergence of posterior expectations to their true values.

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#### MS77

### Stochastic DtN Map, Electrical Impedance Tomography and Boundary Truncation

We address the computational domain truncation problem in electrical impedance tomography. We replace the boundary condition on the truncation boundary with a stochastic Dirichlet to Neumann map. This map is generated by a spatial prior model, such as a Markov random field, over both the domain of interest and the excluded domain. A proper orthogonal decomposition for the discretized stochastic DtN operator is constructed, to yield a decomposition for the operator.

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#### MS77

#### Electrical Impedance Tomography Imaging with Reduced-order Model based on Proper Orthogonal Decomposition

In Electrical impedance tomography (EIT), conductivity distributions are reconstructed based on electrical potential measurements from the boundary. We carry out a model reduction in EIT in the Bayesian framework, using the proper orthogonal decomposition (POD). POD modes for the conductivity and the potential distribution are computed based on the prior model of the conductivity, and sets of POD modes are used as basis functions for the respective distributions. The model reduction reduces computation times remarkably.

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#### **MS77**

#### Methods for Data Reduction in Uncertainty Quantification

A common approach for treating functional responses (e.g. time-dependent or spatially-dependent data) as opposed to scalar responses is to perform principal components analysis and use the principal components in the uncertainty analysis method. This talk will examine the use of autocorrelation time-series models as an alternative method, and compare them with principal components. The methods will be demonstrated on an electrical circuit application.

#### <u>Laura Swiler</u>

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#### **MS78**

#### Randomize-Then-Optimize: a Method for Sampling from Posterior Distributions in Nonlinear Inverse Problems

Many solution methods for inverse problems compute the maximum a posterior (MAP) estimator via the solution of an optimization problem. Uncertainty quantification (UQ), on the other hand, is typically performed using simulation techniques such as Markov chain Monte Carlo. In this talk, we present a Monte Carlo method for UQ, which we call randomize-then-optimize, that makes use of the optimization algorithm used in the MAP estimation step to sample from the posterior density function, even in nonlinear cases.

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#### MS78

# UQ with Edge Location for Quantitative Radiography

In X-ray radiography, Bayesian methods can provide an estimate of the uncertainty in a density profile reconstruction made from a radiograph of an object. One can choose a suitable prior to reconstruct features of interest, but the resultant error bars rely heavily upon this choice. This work introduces a sampling technique for the covariance of an edge-enhancing prior. This novel technique allows one to quantify the uncertainty both in the choice of prior and the resulting reconstruction.

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<u>Michael J. Fowler</u> Clarkson University Department of Mathematics fowlermj@clarkson.edu

#### MS78

#### Point Spread Reconstruction in Radiography

In high energy x-ray radiographic imaging, a problem of interest is the quantitative reconstruction of the point-spread function (PSF) in the standard model for image blur. In this work, we explore a stochastic model for measuring the spread of an edge in a measured image that assumes a priori that the PSF is compactly supported. Via Bayes' Law, we obtain a posterior distribution from which we estimate and quantify the uncertainty for the PSF.

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#### MS78

#### Parameter Estimation in Large Scale State Space Models Using Ensembles of Model Runs

We present a parameter estimation technique targeted to tune closure parameters in large scale operational models used for numerical weather prediction. For those models, existing assimilation systems and model ensemble prediction systems are already available. By adding parameter perturbations to an ensemble systems, we gain information on the parameter uncertainty. The method has been implemented and tested in European Centre for Medium-Range Weather Forecasts (ECMWF).

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#### **MS79**

#### Stochastic Airfoil Model with the Joint Response-Excitation Pdf Approach

We study the stochastic airfoil model based on the limit cycle oscillator by using the joint excitation-response PDF (REPDF) approach. The REPDF evolution equation generalizes the existing PDF equations and enables us to compute the PDF of the airfoil model associated with various types of colored noise. The system consists of two degrees of freedom described by the plunge displacement and the pitch angle. Here we investigate the stochastic solution of this problem induced by the correlated structure of the random forcing and the random initial condition. The REPDF system is solved by the hp-spectral method and the probabilistic collocation method, and algorithm involving separated representation is employed in case of high-dimensions.

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#### **MS79**

#### An Adaptive ANOVA-based Data-driven Stochastic Method for Elliptic PDE with Random Coefficents

In this talk, we present an adaptive, analysis of variance (ANOVA)-based data-driven stochastic method (ANOVA-DSM) to study the stochastic partial differential equations (SPDEs) in the multi-query setting. Our new method integrates the advantages of both the adaptive ANOVA decomposition technique and the data-driven stochastic method. To handle high-dimensional stochastic problems, we investigate the use of adaptive ANOVA decomposition in the stochastic space as an effective dimension-reduction technique. To improve the slow convergence of the generalized polynomial chaos (gPC) method or stochastic collocation (SC) method, we adopt the data-driven stochastic method (DSM) for speed up. An essential ingredient of the DSM is to construct a set of stochastic basis under which the stochastic solutions enjoy a compact representation for a broad range of forcing functions and/or boundary conditions. In our ANOVA-DSM framework, solving the original high-dimensional stochastic problem is reduced to solving a series of ANOVA-decomposed stochastic subproblems using the DSM. An adaptive ANOVA strategy is also provided to further reduce the number of the stochastic subproblems and speed up our method. To demonstrate the accuracy and efficiency of our method, numerical examples are presented for one- and two-dimensional elliptic PDEs with random coefficients.

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#### **MS79**

### Stochastic Modeling of the Land-Air Interface in the Cesm

This work presents a modeling strategy for coupled systems by introducing a stochastic perturbation in the interface. Using collected measurements, the model is tuned using an emulator-based calibration strategy for stochastic simulations. We demonstrate our general strategy by imitating the behavior of the latent heat flux in the land/atmosphere interface for the community earth system model (CESM).

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#### MS79

#### **Bayesian Brittleness**

With the advent of high-performance computing, Bayesian methods are increasingly popular tools for the quantification of uncertainty throughout science and industry. Since these methods impact the making of sometimes critical decisions in increasingly complicated contexts, the sensitivity of their posterior conclusions with respect to the underlying models and prior beliefs is becoming a pressing question. We report new results suggesting that, although Bayesian methods are robust when the number of possible outcomes is finite or when only a finite number of marginals of the data-generating distribution are unknown, they are generically brittle when applied to continuous systems with finite information on the data-generating distribution. This brittleness persists beyond the discretization of continuous systems and suggests that Bayesian inference is generically ill-posed in the sense of Hadamard when applied to such systems: if closeness is defined in terms of the total variation metric or the matching of a finite system of moments, then (1) two practitioners who use arbitrarily close models and observe the same (possibly arbitrarily large amount of) data may reach diametrically opposite conclusions; and (2) any given prior and model can be slightly perturbed to achieve any desired posterior conclusions. This presentation is based on a joint work with Clint Scovel (Caltech) and Tim Sullivan (University of Warwick) and two preprints available online at http://arxiv.org/abs/1304.6772 (H. Owhadi, C. Scovel and T. Sullivan) and http://arxiv.org/abs/1304.7046 (H. Owhadi and C. Scovel).

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#### **MS80**

# An MCMC Algorithm for Parameter Estimation of Partially Observed Signals with Intermittent Instability

Many signals of interest in science and engineering develop intermittency due to nonlinear dynamics with instabilities. A natural way of modeling these signals is through stochastically parameterized models, where intermittency is the outcome of transient instability. Because the stochastic degrees of freedom in this class of models have no direct counterparts with physical observables, traditional data augmentation methods fail to estimate the model parameters. We analyze the failure of the traditional method and propose a new one by preconditioning the unobserved part of the signal. The new method has high prediction skill and is especially successful in capturing intermittency.

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#### **MS80**

#### An Ensemble Kalman Filter for Statistical Estimation of Physics Constrained Nonlinear Regression Models

A central issue in contemporary science is the development of nonlinear data driven statistical-dynamical models for time series of noisy partial observations from nature or a complex model. It has been established recently that ad-hoc quadratic multi-level regression models can have finite time blow-up of statistical solutions and/or pathological behavior of their invariant measure. Recently, a new class of physics constrained nonlinear regression models were developed to ameliorate this pathological behavior. Here a new finite ensemble Kalman filtering algorithm is developed for estimating the state, the linear and nonlinear model coefficients, the model and the observation noise covariances from available partial noisy observations of the state. In this talk, several stringent tests and applications of the method will be discussed. In the most complex application, the perfect model has 57 degrees of freedom involving a zonal (east-west) jet, two topographic Rossby waves, and 54 nonlinearly interacting Rossby waves; the perfect model has significant non-Gaussian statistics in the zonal jet with blocked and unblocked regimes and a non- Gaussian skewed distribution due to interaction with the other 56 modes. We only observe the zonal jet contaminated by noise and apply the ensemble filter algorithm for estimation. Numerically, we find that a three dimensional nonlinear stochastic model with one level of memory mimics the statistical effect of the other 56 modes on the zonal jet in an accurate fashion, including the skew non-Gaussian distribution and autocorrelation decay. On the other hand, a similar stochastic model with zero memory levels fails to capture the crucial non-Gaussian behavior of the zonal jet from the perfect 57- mode model.

#### John Harlim

**MS80** 

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#### Adaptive Sampling

Novel methodologies are presented for optimal Bayesian nonlinear state estimation and adaptive sampling of large nonlinear dynamical systems, both forward and backward in time. The Bayesian nonlinear smoothing is obtained by combining reduced-order Dynamically-Orthogonal (DO) equations with Gaussian Mixture Models (GMMs), extending the backward pass update of the Rauch-Tung-Striebel scheme to a Bayesian nonlinear setting. With this result, a new Bayesian nonlinear adaptive sampling scheme is then derived to predict the observations to be collected that maximize information about variables of interest, in the future and in the past, while accounting for the constraints of the available sensing systems. When combined with our rigorous time-optimal path planning schemes, a unified result is efficient coordinated swarms of autonomous ocean sampling systems.

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#### **MS80**

#### Data Assimilation and Uncertainty Quantification of Co2 Sequestration Process Using Both Fluid Flow and Geo-Mechanical Observation

The application of ensemble-based algorithms for history matching reservoir models has been steadly increasing over the past decade. However, the majority of implementations in the reservoir engineering have dealt only with production data. In reality, however, the production/injection processes may lead to changes in both the flow and geomechanics properties of subsurface reservoir. For example, the injection of CO2 into subsurface reservoir under high pressure/temperature conditions may alter the stress/strain field which may lead to surface uplift or subsidence. In this work, we implement variations of ensemble Kalman filter and ensemmble smoother algorithms for assimilation of both dynamic flow data as well as geomechanical observation data into reservoir model. The results are used to predict and quantify the uncertainty in the movement of CO<sub>2</sub> plume.

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#### **MS81**

Not available at time of publication

Not available at time of publication.

Towards Non-Gaussian Nonlinear Smoothing and

George Biros

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#### MS81

#### **Bayesian Pca for High Dimensional Random Fields**

In this work, we apply classic Bayesian and Approximate Bayesian Computation methods to find principle components for high dimension systems. This Bayesian approach adds a quantifiable uncertainty to the principle components, which is otherwise missing from the classic PCA/ SVD method. The uncertainty around the principle components can be shown to decrease as the number of samples increase, as expected. We also compare this technique to alternate Gaussian Process techniques and look at applications where the dimensionality becomes prohibitive.

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#### MS81

### Massively Parallel PDE Solvers for Uncertainty Quantification

Uncertainty quantification requires the solution of sequences of problems and thus the time to solution for each individual problem may become a critical factor. In parallel computing this translates to strong scaling rather than weak scaling. The talk will present results for the strong scaling of multigrid as solver for elliptic PDE and for the Lattice Boltzmann method for transient flow simulation, together with implications when these methods are used in the UQ context.

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#### MS82

#### Interacting Particle System and Optimal Stopping

The aim of this lecture is to give a general introduction to the interacting particle system and applications in finance, especially in the pricing of American options. We survey the main techniques and results on Snell envelope, and provide a general framework to analyse these numerical methods. New algorithms are introduced and analysed theoretically and numerically.

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#### **MS82**

# Second-Order Bsdes with General Reflection and Game Options under Uncertainty

W extend the results concerning the existence and uniqueness of second-order reflected 2BSDEs to the case of two obstacles. Under some regularity assumptions on one of the barriers and when the two barriers are completely separated, we provide a complete wellposedness theory for doubly reflected second-order BSDEs. We also show that these objects are related to non-standard optimal stopping games, thus generalizing the connection between DRB-SDEs and Dynkin games first proved by Cvitanić and Karatzas (1996). More precisely, we show under a technical assumption that the second order DRBSDEs provide solutions of what we call uncertain Dynkin games and that they also allow us to obtain super and subhedging prices for American game options in financial markets with volatility uncertainty.

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#### MS82

### BSDEs with Markov Chains: Two-Time-Scale and Weak Convergence

This talk is concerned with backward stochastic differential equations (BSDEs) coupled by a finite-state Markov chains with two-time-scale. This kind of BSDEs have wide applications in optimal control and mathematical finance. In particular, it is proved that the solution of the original BSDE system converges weakly under the Meyer-Zheng topology as the fast jump rate goes to infinity.

#### Zhen Wu

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#### MS82

### Approximate FBSDE Using Branching Particle Systems

In this talk, we present an infinite particle system representation for the solutions to a class of forward backward stochastic differential equations. Based on this representation, a numerical approximation to the solutions will be proposed and the convergence rate estimated.

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#### MS83

#### A Scalable MAP-Based Algorithm for Optimal Experimental Design for Large-Scale Bayesian Inverse Problems

We address the problem of optimal experimental design (OED) for infinite-dimensional nonlinear Bayesian inverse problems. We seek an A-optimal design, i.e., we aim to minimize the average variance of a Gaussian approximation to the inversion parameters at the MAP point. The OED problem includes as constraints the optimality condition PDEs defining the MAP point as well as the PDEs describing the action of the posterior covariance. We provide numerical results for the inference of the permeability field in a porous medium flow problem.

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#### MS83

# A Matrix Free Approach for Optimal Experimental Design for Inverse Problems

Goal of the optimal experimental design (OED) is a robust prediction of the model parameters by an appropriate choice of the design of the experiments. Although important developments have been made on numerical methods for OED with differential equations further progresses must be done applying the state-of-the-art approaches for optimization problems constrained with PDE systems. We present an adaptive finite element approach and a matrix free optimization algorithm to solve OED problems in PDE context.

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#### MS83

# Design of Data Collection When Standard DoE Is Not Available

Not available at time of publication.

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#### MS83

#### Fast Bayesian Optimal Design

In [Q. Long, M. Scavino, R. Tempone, S. Wang. CMAME, 2013], a new method based on the Laplace approximation was developed to accelerate the estimation of the post-experimental expected information gains (Kullback-Leibler divergence) in model parameters and predictive quantities of interest in the Bayesian framework. A closedform asymptotic approximation of the inner integral and the order of the corresponding dominant error term were obtained in the cases where the parameters are determined by the experiment. In this work, we extend that method to the general case where the model parameters can not be determined completely by the data from the proposed experiments. We carry out the Laplace approximations in the directions orthogonal to the null space of the Jacobian matrix of the model with respect to the parameters, so that the information gain can be reduced to an integration against the marginal density of the transformed parameters which are not determined by the experiments. Furthermore, the expected information gain can be approximated by an integration over the prior, where the integrand is a function of the posterior covariance matrix projected over the forementioned orthogonal directions. To deal with the issue of dimensionality in a complex problem, we use either Monte Carlo sampling or sparse quadratures for the integration over the prior probability density function, depending on the regularity of the integrand function. We demonstrate the accuracy, efficiency and robustness of the proposed method via several nonlinear under determined test cases. They include the designs of the scalar parameter in an one dimensional cubic polynomial function with two indistinguishable parameters forming a linear manifold, respectively, and the boundary source locations for impedance tomography in a square domain, where the unknown parameter is the conductivity, which is represented as a random field.

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#### MS84

#### Robust Bounds on Risk-Sensitive Functionals Via Renyi Divergence with Applications to Rare Events

In this work, we extend a duality between exponential integrals and relative entropy to Renyi divergence. This formula gives rise to upper and lower bounds that are meaningful for all values of a large deviation scaling parameter, allowing one to quantify, in explicit terms, the robustness of potentially rare events. As applications we consider problems of uncertainty quanti?cation when aspects of the model are not fully known, as well their use in bounding tail properties of an untractable model in terms of a tractable one.

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#### **MS84**

### Statistical Analysis of Extremes and Tail Dependence

Dependence in the tail of the distribution can differ from that in the bulk of the distribution. We will first introduce the framework for describing tail dependence. The probabilistic framework of regular variation has strong ties to classical extreme value theory and provides a framework for describing tail dependence. We will introduce regular variation and the angular measure which fully describes tail dependence. We will then briefly look at two applications which have used this regular variation framework. We examine performing prediction for air pollution given that nearby values are large. And we perform data mining for extremes to determine the meteorological conditions which lead to the most extreme ground level ozone measurements.

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#### MS84

#### Bayesian Discontinuity Detection and Surrogate Construction for Complex Computer Models

Current methods for discontinuity detection often require dense data collection. We propose a Bayesian probabilistic framework to parameterize and infer discontinuities when data or model evaluations are sparse. This formulation leads to a posterior distribution on the discontinuity location which allows the partitioning of parameter space into regions where the model output behaves smoothly. In these regions one can employ efficient spectral representations for model outputs that can be used in subsequent uncertainty quantification studies.

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#### MS84

### A New Class of Stable Processes: Modeling and Bayesian Computation

Not available at time of publication.

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#### MS85

# Numerical Methods with Quantifiable Errors for Astrophysical Simulation

Not available at time of publication.

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#### **MS85**

#### Identification and Diagnostic of Transient Phenomena in Stellar Evolution

Not available at time of publication.

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#### MS85

#### Approximate Sufficiency in Cosmological Estimation Problems

Not available at time of publication.

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#### **MS85**

#### Building the Cosmos: How Simulations Shed Light on the Dark Universe

Not available at time of publication.

#### <u>Risa Wechsler</u>

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#### MS86

#### A Point-Process Approximation to Probability

#### Measures of Spatially Varying Friction Coefficients

We consider a computational measure-theoretic approach to non-parametric inversion of probability measures on physical parameters of a computational model given uncertain quantities of interest. For high dimensional parameter domains, a non-intrusive random sampling approach using results from stochastic geometry is used. A case study for quantifying uncertainty in the spatially varying friction parameters of the ADCIRC model is presented.

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#### $\mathbf{MS86}$

#### Fast Kalman Filters for Seismic Imaging and CO2 Sequestration Monitoring

Tracking the movement of a fluid in the subsurface is a challenge that is often encountered in many applications, such as CO2 sequestration. The numerical algorithms required to process the data are often limited by their high computational cost. We will present HiKF, a new Kalman Filter algorithm that reduces the computational and storage costs. Numerical results show that HiKF can be more accurate than the ensemble Kalman filters (EnKF).

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#### MS86

Scalable Algorithms for Bayesian Inverse Problems and Optimal Experimental Design with Applica-

#### tions to Large-scale Complex Systems

We present scalable algorithms for Bayesian inverse problems and associated optimal experimental design. "Scalable" here refers to computing the relevant solution at a cost that is a constant multiple of the cost of solving the forward problem, independent of problem size. Our algorithms attain scalability due to their exploitation of problem structure in the form of first, second, third, and possibly fourth derivatives of the parameter-to-observable map, for which low-rank approximations are invoked. Applications to ice sheet dynamics of Antarctica are presented.

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#### **MS86**

### Numerical Upscaling Methods for Reservoir Model Reduction

In this talk, we present latest model reduction techniques based on numerical upscaling of multiphase flows for the purpose reliable reservoir performance prediction through rapid uncertainty analysis and data assimilation. From this perspective, the traditional numerical upscaling is relaxed to achieve approximate but fast reduced order models that capture important dynamical features. Numerical tests that demonstrate this approach will be presented.

#### Yahan Yang

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#### MS87

Computational reduction by Reduced Basis Meth-

#### ods for inverse problems governed by PDEs

We present some reduced-order methods (ROMs) to reduce computational complexity of inverse problems, relying on a reduced basis approximation of the state PDE model and, e.g., on a Bayesian framework for uncertainty quantification. Thanks to a suitable Offline/Online computational procedure and a posteriori error estimates, ROMs can provide rapid and reliable solutions to inverse problems governed by linear/nonlinear PDEs.

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#### MS87

### Variable Selection for Quantifying Uncertainty Involving Functional Data

A computer code with one-dimensional functional inputs and a scalar output is studied. The inputs are correlated and have an unknown distribution. The objective of this work is to model these functions. They are decomposed on a basis thanks to a Partial Least Square regression linking the functions and the scalar output. The first few coefficients are selected. The multivariate density of these coefficients is estimated thanks to a sparse Gaussian Mixture model.

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#### MS87

#### Assessing Model Rduction for Sensitivity Analysis

In this talk we firstly motivate the minisymposium by giving a first classification of reduction tools recently proposed for quantifying uncertainties in large-scale problems. We then focus on sensitivity analysis and give some recent developments concerning the reduced basis approach in the context of sensitivity analysis. In order to assess the quality of a sensitivity study based on reduced models it is of great importance to provide certified error bounds.

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#### MS87

#### A Posteriori Error Estimates to Enable Effective Dimension Reduction in Stochastic Systems

Many physical systems have a relatively large number of uncertain parameters. Consequently, understanding how the uncertainty in the parameters propagates through the model to quantities of interest can be a monumental task. In this talk, we show how recently developed error estimates for surrogate models can be used to reduce the effective stochastic dimension for discretized partial differential equations. We demonstrate this methodology using anisotropic refinement for polynomial chaos and sparse grid approximations.

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#### **MS88**

#### Designing Experiments for Optimal Parameter Recovery in Biological Systems

Optimal experimental design can be formulated as a bilevel optimization problem. The inner optimization problem consists of an estimation of model parameter given a certain design. The outer optimization problem minimizes the expected error between recovered and true parameters regarding the design options. We present the empirical Bayes risk problem, investigate computational aspects of the bi-level problem and explore special parameter estimation methods for differential equations. Our framework is illustrated by examples from biomedical applications.

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#### MS88

#### **Online Model Validation**

For differential equation models where the parameters enter nonlinearly, the optimal experimental processing to minimize the parameter uncertainties depends on the parameters values. It is a reasonable approach to recompute the parameter estimates and the controls for the further processing whenever new data has been measured. This method can in particular be applied to processes with parameters varying in time and to processes which have to satisfy boundary conditions. The approach of online parameter estimation and online experimental design has to be applied in a real-time capable implementation. We present numerical methods and application strategies for this task and show examples from chemical engineering and robotics.

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#### MS88

### Robust Optimal Design of Experiments Based on a Higher Order Sensitivity Analysis

When dealing with the task of estimating parameters by the use of a set of noisy data, the number of available measurements is limited. Therefore, in optimum experimental design (doe) it is tried to identify the system settings with those measurements which allow the most reliable estimate. In this talk we are going to present properties and examples of a new and robust doe objective function, which is based on higher order confidence regions.

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#### MS89

#### Local Reduced Order Models for Stochastic Flows and Applications

In this talk, we will discuss some multiscale approaches for solving stochastic problems and their applications to uncertainty quantification in inverse problems. The multiscale methods are based on the generalized multiscale finite element method (GMsFEM) which provides a hierarchy of approximations of different resolution. These hierarchical approximations are used within multilevel Monte Carlo methods. In particular, we describe a multilevel Markov chain Monte Carlo method, which sequentially screens the proposal with different levels of approximations and reduces the number of evaluations required on fine grids, while combining the samples at different levels. The method integrates the multiscale features of the GMsFEM with the multilevel feature of the MLMC methods.

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#### **MS89**

#### Uncertainty Quantification of Coupled Electrochemical Equations for the Simulation of Lithiumion Batteries

The coupled electrochemical governing equations and the fairly large number of random parameters make the uncertainty quantification (UQ) of Lithium-ion batteries (LIB) challenging, specifically when stochastic spectral techniques are employed. In the present study, we propose a fast stochastic approach based on a decoupled formulation of LIB to study the propagation of uncertainties. The proposed decoupling framework alleviates the curseof-dimensionality associated with the UQ of such coupled multi-physics/multi-domain systems.

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#### **MS89**

#### The Stochastic Variational Multiscale Method: A Subgrid Model for Higher-order gPC with an Inbuilt Error Indicator

We present the variational multiscale (VMS) method for stochastic PDEs and apply it to generate accurate coarsescale solutions while accounting for the missing scales through a model term which is defined by a fine-scale stochastic Green's function. We derive an exact expression and an approximation for this Green's function, and explore the possibility of using the resulting fine-scale solution as an error indicator to drive adaptivity in the stochastic space.

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#### **MS89**

Uncertainty Quantification for Coupled Problems

#### in Electronic Engineering

Mathematical modeling of electric machines as well as nanoelectronic devices yields coupled problems. Here differential algebraic equations (DAEs) describe electric networks and partial differential equations (PDEs) specify particular spatial distributed effects like heat dissipation or electromagnetic fields, for example. Coupled systems of DAEs and PDEs can be solved numerically by cosimulation techniques. However, physical parameters of the DAE part and/or the PDE part often exhibit uncertainties because of variability in the manufacturing process. We consider the uncertainties by the introduction of random parameters. For these stochastic models, numerical methods are discussed, which include the structure of the coupled problems in a co-simulation. We present results of simulations for industry relevant problems.

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#### MS90

### Can Small Islands Protect Nearby Coasts from Tsunamis?

Small islands in the vicinity of the mainland are believed to offer protection from wind and waves and thus coastal communities have been developed in these areas. However, what happens when it comes to tsunamis is not clear. Will these islands act as natural barriers ? In this talk, we present a multidisciplinary approach, including modeling the physics, numerical simulations and sequential experimental design under budget constraints, to answer this question.

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#### **MS90**

Propagation of Uncertainties in Tsunami Mod-

#### elling for the Pacific Northwest

VOLNA, a nonlinear shallow water equations solver, produces high resolution simulations of earthquake-generated tsunamis for the Pacific Northwest. Seabed deformations are time-varying shapes difficult to sample; they require an integrated statistical and geophysical analysis. The uncertainties in the bathymetry result from irregularly-spaced observations. We employ sequential designs to efficiently build our Gaussian Process emulator. We propagate source and bathymetry uncertainties to obtain an improved probabilistic assessment of tsunami hazard in this region.

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#### MS90

#### Big Data Methods for Natural Hazard Analysis

Not available at time of publication.

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#### MS90

#### Estimating the Maximum Earthquake Magnitude Based on Background Seismicity and Earthquake Clustering Characteristics

This study aims at getting the best estimate for the largest expected earthquake in a given future time interval and spatial region from a combination of historic and instrumental earthquake catalogs, based on the ETAS (epidemictype aftershock sequence) model, where the Gutenberg-Richter law for earthquake magnitude distribution cannot be directly applied.

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#### MS91

# On the Role of Wind Correlation in Power Grid Stochastic Optimization Models

The effects of improper estimation of the covariance matrix between wind farms on the optimal dispatch in power grid systems are investigated. We present analytic results and large scale computer simulations which indicate that over/underestimation of correlation leads to higher operating costs, and, potentially, to market inefficiencies in electrical power grids.

#### Cosmin G. Petra

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#### MS91

#### Probabilistic Density Function Method for Stochastic Odes of Power Systems with Uncertain Power Input

Wind and solar power generators are commonly described by a system of stochastic ordinary differential equations. The existing methods for SODEs are mostly limited to delta-correlated random parameters (white noise). Here we use the Probability Density Function method for deriving a closed-form deterministic partial differential equation (PDE) for the joint probability density function of the SODEs describing a power generator with time-correlated power input.

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#### MS91

## Approximating Stochastic Process Models for Load and Wind Power in Stochastic Unit Commitment

This talk describes work that is part of a large ARPA-e project on stochastic unit commitment, to optimize dayahead and intra-day electricity generation plans taking into account the uncertainty provided by both load and the high use of renewables. We will discuss some optimization problems that result from creation of stochastic process models for load and available renewable energy. We will also discuss the extraction of probabilistic scenarios from the stochastic process models and evaluation of those scenario sets for use in the stochastic programming model.

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#### MS91

#### Gaussian Process Modeling with Incomplete Data: Applications to Building Systems

We present an implementation of a Monte-Carlo Expectation Maximization (MCEM) algorithm for training a Gaussian Process (GP) under input uncertainty and discuss applications in building systems.

<u>Victor Zavala</u> Argonne National Laboratory vzavala@mcs.anl.gov

#### MS92

#### Forward Backward Doubly Stochastic Differential Equations and Applications to The Optimal Filtering Problem

We consider the classical filter problem where a signal process is modeled by a stochastic differential equation and the observation is perturbed by a white noise. The goal is to find the best estimation of the signal process based on the observation. Kalman Filter, Particle Filter, Zakai equations are some well known approaches to solve optimal filter problems. In this talk, we shall show the optimal filter problem can also be solved using forward backward doubly stochastic differential equations. Both theoretical results and numerical experiments will be presented.

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#### MS92

### Runge-Kutta Schemes for Backward Stochastic Differential Equations

We study the convergence of a class of Runge-Kutta type schemes for BSDEs in a Markovian framework. The schemes belonging to the class under consideration benefit from a certain stability property. As a consequence, the overall rate of convergence of these schemes is controlled by their local truncation error. Under sufficient regularity on the final condition and on the coefficients of the BSDE, we prove high order convergence rate. We also discuss order barriers.

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#### MS92

### Stochastic Control Systems Driven by Fractional Brownian Motions With Hurst Index $H_{L1/2}$

We obtain a maximum principle for stochastic control problem of general controlled stochastic differential systems driven by fractional Brownian motions (of Hurst index H $_{L1}/2$ ). We introduce a type of backward stochastic differential equations driven by both fractional Brownian motions and the corresponding underlying standard Brownian motions to specify the necessary condition that the optimal control must satisfy. Our approach is to use conditioning and Malliavin calculus.

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#### MS92

A Stochastic Approach Via FBSDEs for Hyperbolic Conservation Laws

By adopting such formula nonlinear Feynman-Kac formula, we consider in this work a new accurate approach for the hyperbolic conservation laws via FBSDE. This relies on solving an equivalent forward backward stochastic differential equation. It is noticed that in such framework, one does not need to handle the discertizations of derivatives and the transition layers, and high accuracy viscosity solution can be found. Several numerical examples are given to demonstrate the effectiveness and accuracy of the proposed numerical method.

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#### **MS93**

### Robust Optimization with Chance Constraints in Noisy Regimes

We present a provably convergent optimization approach for constrained optimization subject to two sources of uncertainties. The first is inherent to the constraints and objective function. The second source of uncertainty stems from computational inaccuracies in the function evaluations. We introduce a derivative free robust optimization approach based on path-augmented constraint approximations. Furthermore, we propose an indicator for detecting inaccurate and noisy function evaluations to prevent corruption of the optimal point.

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#### MS93

#### Uncertainty Quantification in DPD Simulations by Applying Compressive Sensing

We investigate the way to optimize the force field in the dissipative particle dynamics (DPD) model in mesoscopic simulations. We propose a method to quantify the distribution of the force parameters within certain confidence range via Bayesian inference. We employ compressive sensing method to compute the coefficients in the generalized polynomial chaos (gPC) expansion, which is a surrogate model of DPD, given the prior knowledge that the coefficients are "sparse".

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#### **MS93**

### Uncertainty Quantification of Dynamic Systems with Periodic Potentials

Increasing renewable energy production is deemed a priority in President Obama's second term but its large spatiotemporal variation and uncertain nature pose great challenge to our existing power grid. To aid decision making for grid stability, we propose a new uncertainty quantification method to obtain full statistical information of the system states for power systems driven by colored noise (fluctuations with finite correlation time). Having obtained an analytical expression for the system distribution at stationary state, we conduct sensitivity analysis that concerns system stability at large time.

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#### **MS94**

#### Evaluation of Real Gas Effects in Multiphase Flows Using Bayesian Inference and Uncertainty Quantification

We are interested in the simulation of non mixable multiphase flows. Each phase has its own equation of state, and are coupled via interface and relaxation terms that mimic drag, acoustic effects, etc. We present a numerical model coupling a numerical scheme for compressible multiphase flows, a semi intrusive UQ methodology and Bayesian inference in order to calibrate the equation of state. Application to expansion shocks will be presented.

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#### MS94

# Bayesian Model Average Estimates of Turbulence Closure Error

We obtain stochastic estimates for the error in Reynolds-Averaged Navier-Stokes (RANS) simulations due to the closure model, for a limited class of flows. In particular we search for estimates grounded in uncertainties in the space of model closure coefficients, which we estimate for a range of scenarios and closure models using Bayesian calibration. Bayesian model averaging, with adaptive chosen scenario weights, is then used to construct a posterior predictive distribution for an unseen flow.

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#### MS94

#### Quantification of Model-Form Uncertainty in Turbulence Closures

The inability of Reynolds-averaged Navier-Stokes simulations with linear eddy viscosity models to predict flow separation and reattachment limits the reliability of such simulations in engineering problems. We consider the flow over a wavy wall and describe a methodology based on perturbing the Reynolds stresses. This approach correctly estimates the uncertainty in the location of the reattachment point along the wavy wall. We present comparisons of predictions using the SST k-omega and the realizable k-epsilon model.

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#### MS94

Quantification of Model-Form Uncertainties in Thermodynamic Models for Dense Gas Flows

Dense gas flows, of common use in many engineering ap-

plications, strongly deviate from the classical perfect gas behavior. As a consequence, advanced equations of state (EOS) must be used whose coefficients are often ill-known and difficult to obtain experimentally. We use Bayesian techniques to calibrate several EOS applied to the simulation of a dense gas flow around a NACA0012 airfoil, and BMA to quantify uncertainties associated with the mathematical structure of EOS.

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#### MS95

#### Computational Techniques for Experimental Design for Ill-Posed Problems

Design for inverse problems is a delicate matter. Either the prior or the bias needs to be carefully estimated in order to have a realistic design. In this talk we discuss methods for the estimation of the prior and show how this could be used in the context of Bayesian design. In particular, we discuss the estimation of the (inverse) covariance matrix for large scale problems using efficient optimization and linear algebra techniques.

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<u>Eldad Haber</u> Department of Mathematics The University of British Columbia haber@math.ubc.ca

#### MS95

#### Bayesian Experimental Design for the Identification of Stochastic Reaction Dynamics

Although single-cell techniques are advancing rapidly, quantitative assessment of kinetic parameters is still characterized by ill-posedness and a large degree of uncertainty. For traditional protocols the information gain between subsequent experiments or time points is comparably low, reflected in a hardly decreasing parameter uncertainty. Here we introduce a framework to design optimal perturbations for the inference of stochastic reaction dynamics. We maximize the information gain as characterized by the distance between posterior and prior distribution.

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#### MS95

#### Optimum Experimental Design for Partial Differential Equations

A common technique to reduce parameter uncertainties in complex models - possibly consisting of PDEs - is to use optimum experimental design. Therefor second mixed order derivatives are required when using derivative based optimization methods. For accurate computation we use automatic differentiation acting on local residuals. Robust simulation is important, especially when it comes to infeasible path methods. Results for charge transport in disordered organic semiconductors are presented along with stabilization and damping strategies for Gummel's method.

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Andreas Schmidt Interdisciplinary Center For Scientific Computing, Heidelberg Andreas.Schmidt@iwr.uni-heidelberg.de

#### MS96

#### Probabilistic Approaches for Fault-Tolerance and Scalability in Extreme-Scale Computing

We present a novel approach for solving PDEs, using a probabilistic representation of uncertainty in the PDE solution due to incomplete convergence and the effect of system faults. Using domain decomposition, the problem is reduced to solving the PDE on subdomains with uncertain boundary conditions. An iterative approach to solve this problem in a resilient and scalable way, using subdomain computations for sampled values of the subdomain boundary conditions, is demonstrated on elliptic systems.

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#### MS96

The Computational Complexity of Stochastic Galerkin and Collocation Methods for PDEs with

#### **Random Coefficients**

We developed a rigorous cost metric, used to compare the computational complexity of a general class of stochastic Galerkin methods and stochastic collocation methods, when solving stochastic PDEs. Our approach allows us to calculate the cost of preconditioning both the Galerkin and collocation systems, as well as account for the sparsity of the Galerkin projection. Theoretical complexity estimates will also be presented and validated with use of several computational examples.

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#### **MS96**

#### Resilient Sparse Representation of Scientific Data for Uq on High Performance Computing

Not available at time of publication.

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#### MS96

#### Exploring Emerging Manycore Architectures for Uncertainty Quantification Through Embedded Stochastic Galerkin Methods

We explore approaches for improving the performance of embedded stochastic Galerkin uncertainty quantification methods on emerging computational architectures. Our work is motivated by the trend of increasing disparity between floating-point throughput and memory access speed. We describe several new stochastic Galerkin matrix-vector product algorithms and measure their performance on contemporary manycore architectures. We demonstrate these algorithms lead to improved memory access patterns and ultimately greater performance within the context of iterative linear system solvers.

#### Eric Phipps

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#### **MS97**

### A Probabilistic Method for Efficient Behavior Classification

Parameter synthesis, or behavior classification, is the problem of identifying the set of parameters for which a given system satisfies a given condition. We describe two sampling schemes and a method to use these samples to produce a probability distribution on curves in order to approximate the boundary of the parameters satisfying the given condition. We provide both theoretical and numerical results illustrating the effectiveness of our method, even in the case that the boundary has multiple components.

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#### MS97

#### Stochastic Multiscale Analysis: a Benchmark Study in Materials Systems

This research uses benchmark computational studies to unveil scenarios where uncertainties significantly affect macroscopic material behavior. The numerical experiments capture the main features of a wide class of problems in materials. The generalized uncertainty propagation criterion whose assessment may be used to understand whether uncertainties may non-negligibly propagate to apparent system properties, combines four features of a microstructured material system: the microstructure size (micro), material property correlation length (micro), structure size (macro), and global length scale of loading (macro).

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#### MS97

### Random Discrete Least Square Polynomial Approximation for Pdes with Stochastic Data

We consider a PDE with random parameters and analyze the least squares method for polynomial approximation of the solution based on random sampling of the parameters. In particular we discuss the stability and optimality of the random least squares method in arbitrary dimension depending on the size of the random sample and the dimension of the polynomial space. We also discuss greedy type adaptive algorithms for the selection of the polynomial space.

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#### **MS97**

#### A Probabilistic Graphical Model Approach to Uncertainty Quantification for Multiscale Systems

We present a probabilistic graphical model for uncertainty quantification in multiscale/multiphysics systems. This representation provides explicit factorization of the highdimensional joint probability distribution. Hidden variables are naturally introduced to capture the effect of fine scale variables on coarse grained responses. The hyperparameters in the probabilistic model are learned using sequential Monte Carlo (SMC) method. We make predictions from the probabilistic graphical model using belief propagation algorithms. This framework addresses many of the difficulties of current UQ methods including among others (a) modeling of correlations, multi-outputs, time/space responses; (b) efficient inference using belief propagation algorithms; (c) modeling of epistemic uncertainty and (d) allowing data from multiple sources. Numerical examples are presented to show the potential of such approaches in solving stochastic multiscale/multiphysics PDEs.

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#### **MS98**

#### Improved and Fast Gasp Emulation Strategies

UQ analyses are often based on fast approximations (surrogates) to computer (math) models . GasP Gaussian Processes are perhaps the most used because the computations are relatively simpler. We show how the usual fitting can be seriously unsuitable and provide better alternatives still giving closed form expressions. However UQ analyses with Gasp can still be unfeasible for really complex and/or large problems. Use of fast parallel partial emulation with adaptive sub-design is recommended.

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#### MS98

# Where Are You Gonna Go When the Volcano Blows?

Hazards consequent to volcanic explosions include hot, ground-hugging pyroclastic flows that can race along at speeds up to 50m/sec, and ash plumes that rise into the atmosphere and can wreck havoc with air traffic. Computer simulations of mathematical models of these volcanic phenomena are expensive to run. Using a combination of careful analysis and statistical methodology, together with expert and a limited number of computer simulations, enough data can be collected to make quantifiable, statistically accurate predictions of the hazard. Indeed, with enough care a hazard map can be made describing areas of relatively higher and lower risk. This talk will review some of the mathematics, statistics, and geology needed to compute the hazard risk.

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#### **MS98**

### Combinbing Multiple Sources of Uncertainty in Geophysical Hazard Mapping

Should you worry about your pde solver's numerical error if there is uncertainty in parameters, initial conditions, boundary conditions, etc? Presumably if you ask this question, your solver is computationally expensive and you hope the answer is "no." In the context of geophysical haz-

ard mapping, we propose a surrogate-based methodology which efficiently assesses the impact of various uncertainties enabling a quick yet methodical comparison of the effects of uncertainty and error on computer model output.

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#### $\mathbf{MS98}$

#### Parallel Thinning

Many statistical methods break down with copious data: likelihoods become peaked; MCMC mixes slowly, inference becomes impractical. Our new variation on parallel tempering, for ID-distributed data, uses parallel Markov chains constructed with stationary densities proportional to likelihoods for p-thinned data for a range of p, linked to original by occasional "swap' moves. Thinned chains' rapid mixing accelerates convergence in original chain. For both simulated and astronomical data, we attain accelerated convergence in otherwise intractable problems.

Robert L. Wolpert, Mary E. Broadbent

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#### MS99

#### Scalable Gaussian Process Analysis

We discuss the problem of parameter estimation for Guassian Process models of random fields. Classical approaches require the Cholesky factorization of a possibly dense covariance matrix for the purpose of computing the log-determinant terms; which is not tenable for emerging large-scale applications when millions to billions of data points are involved and thus dense matrices with  $10^{12}$ - $10^{18}$  elements would need to be factorized. We present a stochastic approximation approach to the maximum likelihood estimation that, under some conditions produces an estimate whose error is comparable to the one of the exact likelihood estimator itself and which reduces the calculations to linear solves with the covariance matrix. We demonstrate the scalability potential of the method with synthetic and measured data sets.

#### <u>Mihai Anitescu</u>

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#### MS99

Dakota Infrastructure and Algorithms Enabling Advanced UQ

UQ methods typically require a judicious choice of many long-running but modestly-sized simulations. Thus, it is important to manage their assignment to large-scale computational resources in an effective manner. We will give an overview of several advanced UQ algorithms in Dakota, a multilevel parallel object-oriented framework for parametric analysis, and describe the parallel infrastructure that enables their execution on HPC platforms. We will also discuss examples that demonstrate the interplay between UQ methods and parallelism.

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#### MS99

### Statistical Inversion for Basal Parameters for the Antarctic Ice Sheet

We formulate a Bayesian inference problem for the friction field at the base of the Antarctic ice sheet from distributions for the observed surface velocities and for the prior knowledge of the basal friction. The dimension of the parameter space is large, and the map from parameters to observations requires the solution of a system of implicit nonlinear 3D PDEs. We approximate the posterior distribution with a Gaussian centered at the maximum a posteriori point, with covariance given by the inverse Hessian of the log posterior. By using a low-rank approximation of the log likelihood, we are able to scale up to the problem size of interest.

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#### $\mathbf{MS99}$

#### Advances and Challenges of Uncertainty Quantification with Application to Climate Prediction

In this talk, I will focus on 3 research efforts in UQ (i) Error Estimation in multi-physics and multi-scale codes; (ii) Tackling the Curse of High Dimensionality; and (iii) development of an advanced UQ Computational Pipeline enabling UQ workflow and analysis for ensemble runs at the extreme scale (e.g. exascale) with self-guiding adaptation in the UQ Pipeline engine. Applications to the quantification of uncertainty associated with Climate prediction will be addressed.

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#### $\mathbf{MS100}$

#### Value in Mixed Strategies for Zero-Sum Stochastic Differential Games Without Isaacs Condition

We consider 2-person zero-sum stochastic differential games with a non-linear pay-off functional defined through a backward stochastic differential equation. Our main objective is to study for such a game the problem of the existence of a value without Isaacs condition.

#### <u>Juan Li</u>

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Rainer Buckdahn, Marc Quincampoix Universit e de Brest marc.quincampoix@univ-brest.fr, marc.quincampoix@univ-brest.fr

#### MS100

#### Stochastic Control Representations for Penalized Backward Stochastic Differential Equations

We show that penalized BSDE, which is often used to approximate and solve the corresponding reflected BSDE, admits both optimal stopping representation and optimal control representation. The new feature of the optimal stopping representation is that the player is allowed to stop at exogenous Poisson arrival times. We then apply the representation results to two classes of equations, namely multidimensional reflected BSDE and reflected BSDE with a constraint on the hedging part, and give stochastic control representations for their corresponding penalized equations.

Gechun Liang University of Oxford liangg@maths.ox.ac.uk

#### $\mathbf{MS100}$

#### Split-step Milstein Methods for Multi-channel Stiff Stochastic Differential Systems

We consider a family of split-step Milstein methods for the solution of stochastic differential equations with an emphasis on systems driven by multi-channel noise. We show their strong order of convergence and investigate mean-square stability properties for different noise and drift structures. The stability matrices are established in a form convenient for analyzing their impact arising from different deterministic drift integrators. Numerical examples are provided to illustrate the effectiveness and reliability of these methods.

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#### **MS100**

### Robust Utility Maximisation Via Second Order BSDEs

The problem of robust utility maximisation in an incomplete market with volatility uncertainty is considered, in the sense that the volatility of the market is only assumed to lie between two given bounds. The set of all possible models (probability measures) considered here is non-dominated. We propose studying this problem in the framework of second order backward stochastic differential equations (2BSDEs for short) with quadratic growth generators. We show for exponential, power and logarithmic utilities that the value function of the problem can be written as the initial value of a particular 2BSDE and prove existence of an optimal strategy. Finally several examples which shed more light on the problem and its links with the classical utility maximization one are provided. In particular, we show that in some cases, the upper bound of the volatility interval plays a central role, exactly as in the option pricing problem with uncertain volatility models.

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#### $\mathbf{PP1}$

### Fuzzy Solution of Interval Linear Programming with Fuzzy Constraints

In many applications of linear programming, the problem coefficients cannot be determined in a precise way. The difficulty of this method lies in the fact that while dealing with such problems it is not clear what the optimal solution is. This paper presents some consideration when solving the linear programming problems with interval coefficients in the constraints. We focus on fuzzy linear prom ramming problem. We derive a new method to solve linear programming problems in the fuzzy sense.

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#### PP1

#### Multilevel Monte Carlo Simulation for Stochastic Models in Chemical Kinetics

With MLMC we simulate a relatively small number of sample paths to get an approximation of the total paths necessary for a given confidence interval and to determine the optimal number of paths per level that minimizes runtime. Here we use total step count as the quantity of interest to optimize the size of random number batches in the full simulation. We then perform sensitivity analyses on the stochastic model and implement on GPU.

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#### PP1

Sensitivity Analysis of Models with Dynamic Inputs

#### Application to the Impact of the Weather Data on the Performance of Passive Houses

We address the issue of performing UASA with two kinds of uncertain inputs, static and dynamics. The originality of the proposed approach is to separate the random variable of the dynamic inputs, propagated to the model response, from the deterministic spatio/temporal function, using Karhunen-Loève decomposition of the dynamic inputs. The approach is applied to a building energy model, in order to quantify the impact of the weather data on the performance of a real passive house.

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#### PP1

#### Evaluation of Some Estimators for Arrival Rate and Probe Proportion in Queue Length Estimation Problem

The research compares the developed primary parameter estimators of the arrival rate  $\lambda$  and probe proportion p at traffic signals using some of the fundamental information (e.g., location, time, and count) that probe vehicles (i.e., vehicles equipped with GPS and wireless communication technologies) provide. For a single queue with Poisson arrivals, analytical models are developed to evaluate how estimation error changes as percentage of probe vehicles in

the traffic stream varies.

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#### PP1

#### An Adaptive Change Point Based Prediction Model: Application to Transportation Networks

This study develops a method for predicting system parameters under abrupt changes or sudden shifts based on an adaptive Hidden Markov Model (HMM) and Time Series ARIMA Models. An approach of employing change point models at these shifts has been taken to switch prediction models. Transition matrix in HMM is adapted by a model on magnitude and duration of the change. The model is evaluated using the California PATH 1993 I-880 database.

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Charles Taylor Norfolk State University charlesmlb53@yahoo.com

#### $\mathbf{PP1}$

#### Analysis of Some Arrival Distributions for Queue Length Estimation Problem

This research focuses on queue length estimation problem at an isolated traffic intersections. The study contributes by embedding the bunching effect of traffic. Arrival distributions from the literature such as Negative Binomial, Generalized Poisson, Geometric Bunch, Inflated-parameter Poisson, Cowan M3, and Poisson are incorporated. The accuracy of the estimation models at various arrival rates is explored.

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#### PP1

#### Uncertainty Quantification for Airfoil Icing Using Polynomial Chaos Expansions

This work aims to quantify the uncertainty that arises in airfoil aerodynamic performance metrics (eg. stall angle of attack) due to uncertainty in the physical process of airfoil ice accretion. This is achieved using Polynomial Chaos Expansions (PCE). We discuss how these PCE surrogate models may be used in a Bayesian parameter estimator to deduce the presence of dangerous airfoil ice shapes in flight, based on a series of noisy measurements of aerodynamic performance metrics.

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#### PP1

#### A Fractal Model of Time

In traditional quantum mechanics, time is considered to be an observable; no time operator has been established. One of the most familiar results of quantum mechanics is the quantization of energy. Inherent in Planck's constant, with its units of time multiplied by energy, lies the concept of the quantization of time. For a certain class of state functions, time can be quantized in time-energy quanta, based upon the existence of a family of quantum-mechanical time operators. These time operators would be a function of the Hamiltonian, the energy operator, and yield nine results for each energy level. The applications of this model include high energy fusion and cosmology. However, our results are entirely theoretical, and have to be confirmed with a real system, such as a hydrogen atom. The question of whether time can be quantized or no is more than academic. If such quantization can be verified, it might serve as a basis for a complete unified field theory.

Jorge Diaz-Castro

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#### PP1

#### A Scalable, Adaptive, Hessian-Based Gaussian Mixture Proposal for Large-Scale Statistical Inverse Problems, with Applications to Subsurface Flow

We address the challenge of large-scale nonlinear statistical inverse problems by developing a Hessian-based Gaussian process surrogate and a Gaussian mixture, both approximating the posterior pdf solution. We employ an adaptive sampling strategy for exploring the parameter space to build these surrogates. The Gaussian mixture approximation is used as a proposal for sampling both the surrogate and the true posterior. The accuracy and efficiency of the algorithms are demonstrated for a subsurface flow problem.

H. Pearl Flath

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#### PP1

#### Impacts of Greenland Surface Mass Balance Uncertainties on Ice Sheet Initialization and Predictions of Sea Level Rise in 2100

Within a coupled climate model, ice sheet boundary conditions are subject to biases from other components of the earth system. We are interested in understanding how large such biases can be before they have an impact on estimates of sea level rise between now and 2100. Here we evaluate how errors in Greenland surface mass balance affect scatter in sea level rise projections using the Community Ice Sheet Model.

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#### PP1

#### Adapting Actuated Traffic Signal Control Settings with Queue Lengths from Probe Vehicles

This study presents a method that adjusts maximum green times in an actuated signal control based on the queue lengths obtained from probe vehicle data. The method is tested on a single intersection with random arrivals, and evaluated in a microscopic traffic simulation environment, and C++ simulations. The queue length-based method provides significant improvements in efficiency. On average % 51 to % 83 decrease in queue lengths are achieved for major and minor streets respectively.

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#### PP1

### Uq of Computational Fluid Dynamics Models in Nuclear Applications

This poster will discussion UQ application in industrial simulations.

<u>Jordan Ko</u> AREVA NP

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#### PP1

### Uncertainties Propagation and Estimation of a Quantile

Our aim is to estimate the quantile of the distribution Y = f(X) where f is an expensive-to-evaluate function. As the Stepwise Uncertainty Reduction strategy is powerful but not numerically tractable, we develop another method : we choose a sequential design such that the next point where f is evaluated minimizes an error built on an estimator of the true quantile. This strategy is numerically better because the criteria has a closed-form thanks to Kriging update formulae.

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#### PP1

### Matrix-Free Geostatistical Inversion with An Application in Large-Scale Hydraulic Tomography

Geostatistical approaches are widely used for inverse problems in geosciences. However, the Jacobian matrix needs to be computed from  $\min(m,n)$  forward runs for m unknowns and n observations, which can be prohibitive when m and n become large. We present and compare "matrixfree" implementations that perform a smaller number of forward runs. The approximation of the prior covariance with controlled accuracy using discrete cosine transform or randomized Eigen-decomposition works well as illustrated in a large-scale Hydraulic Tomography problem.

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#### PP1

#### Symmetry in Quantum Turbulence

Turbulence is a phenomenon associated with chaotic and stochastic change in properties. The unpredictability of natural disasters such as hurricanes and tornadoes is due to turbulence in weather patterns. At the quantum level, turbulence can be found in quantum fluids also known as super fluids; a friction free state of matter containing charged particles. Super fluidity has recently been observed at the core of neutron stars. These fluids containing charged particles also act as perfect electrical conductors that never lose energy (superconductors). This study employs the non-linear Schrodinger coupled with Poissons equation for three dimensional quantum turbulence simulations. Research has found evidence of soliton solutions to the non-linear Schrodinger coupled with Poissons equation. Solitons are self-reinforcing waves in nature that are also symmetric. Future research involves finding solutions to the NLS for a dynamic model.

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#### $\mathbf{PP1}$

#### Balanced Split-Step Methods for Stiff Multiscale Stochastic Systems with Uncertainties

We present split-step balanced methods for the solution of stochastic differential equations with multichannel noise arising in chemical systems which involve reactions at different time scales and change stiffness with uncertainty. We also discuss stochastic destabilization due to the presence of mutually independent multiple Wiener perturbations. For these methods, we propose optimal parameter selection with respect to the desired convergence, stability and positivity properties. Numerical examples are provided to show the effectiveness of these methods.

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#### PP1

## Using Emulators and Hierarchical Models for UQ in Hazard Forecasting

We are developing computationally fast statistical emulators of a computer model of pyroclastic flows. These emulators are very flexible from an uncertainty modeling point of view. Our goal is to use these emulators in conjunction with a hierarchical model to improve our prediction of hazardous events related to these flows. This approach will enable us to combine our results from previously studied sites and gain some knowledge on new locations as they become of interest.

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#### PP1

#### Applications of Statistical Inference in the Design of High-Performance Optical Metamaterials

Bayesian inference and Markov Chain Monte Carlo based methods have been successfully used to approach inverse problems where numerically generated data is readily available. We apply these methods to wave-propagation problems where properties of the initial condition and propagation media are unknown or uncertain. Ultimately, this statistical inversion gives us a means to design plasmonic metamaterials with experimentally desirable optical properties.

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#### PP1

# Regularized Collocation for Spherical Harmonics Gravitational Field Modeling

Motivated by the problem of satellite gravity gradiometry, which is the reconstruction of the Earth gravity potential from the satellite data provided in the form of the secondorder partial derivatives of the gravity potential at a satellite altitude, we discuss a special regularization technique for solving this severely ill-posed problem in a spherical framework. We are especially interested in the regularized collocation method. As a core ingredient we present an a posteriori parameter choice rule, namely the weighted discrepancy principle, and proves its order optimality. Finally, we illustrate our theoretical findings by numerical results for the computation of the Fourier coefficients of the gravitational potential directly from the noisy satellite data.

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#### Valeriya Naumova

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# Notes

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# SIAM Conference on UNCERTAINTY QUANTIFICATION

March 31-April 3, 2014 Hyatt Regency Savannah Savannah, Georgia, USA

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Oberai, Assad, MS89, 3:00 Thu Oduola, Cassandra, PP1, 8:00 Mon Oliver, Todd, MS29, 10:30 Tue Onwunta, Akwum, CP18, 3:00 Thu

### Ρ

Packard, Andrew, MS63, 3:30 Wed Papaspiliopoulos, Omiros, MS50, 6:00 Tue Papaspiliopoulos, Omiros, MS72, 5:30 Wed Parker, Albert, MS68, 3:00 Wed Parker, Robert, IP7, 8:15 Thu Parno, Matthew, MS26, 11:00 Tue Patra, Abani K., MS90, 2:00 Thu Patra, Abani K., MS90, 3:30 Thu Patra, Abani K., MS98, 4:30 Thu Peherstorfer, Benjamin, MS58, 9:30 Wed Peherstorfer, Benjamin, MS58, 9:30 Wed Peng, Ji, CP10, 2:00 Tue Perdikaris, Paris, MS45, 6:00 Tue Pereverzyev, Sergei, MS3, 9:30 Mon Perez, Ricardo, CP17, 3:00 Thu Perrin, Guillaume, CP11, 5:30 Tue Petra, Cosmin G., MS91, 3:30 Thu Petra, Noemi, MS7, 9:30 Mon Petra, Noemi, MS7, 11:00 Mon Pettersson, Mass Per, CP14, 3:40 Wed Pflüger, Dirk, MS35, 2:00 Tue Pflüger, Dirk, MS44, 4:30 Tue Pflüger, Dirk, MS58, 9:30 Wed Pflüger, Dirk, MS81, 9:30 Thu Pflüger, Dirk, MS99, 4:30 Thu Phipps, Eric, MT8, 2:00 Thu Phipps, Eric, MT8, 2:00 Thu Phipps, Eric, MS96, 4:30 Thu Phipps, Eric, MS96, 4:30 Thu Pitman, E. Bruce, MS98, 4:30 Thu Plechac, Petr, MS62, 2:00 Wed Plechac, Petr, MS62, 2:30 Wed Plechac, Petr, MS72, 4:30 Wed Plumlee, Matthew, MS8, 9:30 Mon Plumlee, Matthew, MS25, 5:00 Mon Plumlee, Matthew, MS25, 4:30 Mon

Plumlee, Matthew, MS79, 10:00 Thu Pratola, Matthew T., MS4, 10:30 Mon *Prieur, Clémentine, MS87, 9:30 Thu* Prieur, Clémentine, MS87, 9:30 Thu Pulch, Roland, MS89, 2:30 Thu

Qi, Di, MS14, 3:30 Mon Qian, Peter, MS8, 9:30 Mon Qian, Peter, MS25, 4:30 Mon Qian, Peter, MS8, 10:30 Mon

### R

Rai, Prashant, MS39, 2:30 Tue Ram, Parikshit, MS58, 10:30 Wed Ray, Jaideep, MS29, 9:30 Tue Ray, Jaideep, CP14, 3:20 Wed Reese, Shane, MS25, 5:30 Mon Regayre, Leighton, MS22, 5:00 Mon Rempala, Greg, MS52, 10:30 Wed Ren, Weiging, MS11, 3:00 Mon Reshniak, Viktor, PP1, 8:00 Mon Reshniak, Viktor, MS100, 6:00 Thu Restrepo, Juan M., MS61, 3:30 Wed Ridzal, Denis, MS30, 9:30 Tue Rochinha, Fernando A., CP13, 10:30 Wed Roderick, Oleg, MS12, 2:30 Mon Roemer, Ulrich, CP8, 10:30 Tue

Rosic, Bojana V., CP1, 10:10 Mon RoyChowdh, Sayak, MS60, 3:00 Wed *Rozza, Gianluigi, MT3, 9:30 Tue* Rozza, Gianluigi, MT3, 9:30 Tue *Rozza, Gianluigi, MS45, 4:30 Tue* Ruede, Ulrich J., MS81, 10:00 Thu Russell, Brook, MS84, 11:00 Thu Rutarindwa, Regis, PP1, 8:00 Mon

#### S

S.R. Sri.R. Srinivasa Rao, Arni, MS52, 9:30 Wed S.R. Sri.R. Srinivasa Rao, Arni, MS52, 11:00 Wed Sacks, Jerome, IP4, 1:00 Tue Safta, Cosmin, MS84, 10:30 Thu Saibaba, Arvind, MS37, 2:00 Tue Saibaba, Arvind, MS46, 4:30 Tue Saibaba, Arvind, MS46, 4:30 Tue Sain, Stephan, MS5, 10:30 Mon Samanta, Amit, MS75, 5:00 Wed Samulyak, Roman, MS36, 2:30 Tue Sanderson, Ben, MS5, 10:00 Mon Sang, Huiyan, MS13, 3:00 Mon Santitissadeekorn, Naratip, MS27, 10:30 Tue Sanz-Alonso, Daniel, MS27, 9:30 Tue Sapsis, Themistoklis, MS6, 9:30 Mon Sapsis, Themistoklis, MS6, 10:00 Mon Sapsis, Themistoklis, MS14, 2:00 Mon Sapsis, Themistoklis, MS23, 4:30 Mon Sapsis, Themistoklis, MS28, 10:30 Tue Sargsyan, Khachik, MS39, 2:00 Tue Schaefer, Tobias, MS11, 2:00 Mon Schaefer, Tobias, MS11, 3:30 Mon Schaefer, Tobias, MS20, 4:30 Mon Schafer, Chad, MS85, 5:30 Thu Scheichl, Robert, MS9, 3:30 Mon Scheichl, Robert, MS69, 4:30 Wed Schick, Michael, CP14, 2:40 Wed Schillings, Claudia, MS34, 3:30 Tue Schlegel, Nicole-Jeanne, MS7, 10:30 Mon Schmidt, Christian, CP12, 5:50 Tue

Schneider, Reinhold, MS48, 6:00 Tue Schulze-Riegert, Ralf, MT5, 9:30 Wed Schulze-Riegert, Ralf, MT5, 9:30 Wed Seppanen, Aku, MS77, 5:30 Wed Singla, Puneet, MS38, 3:00 Tue Sinsbeck, Michael, MS35, 3:00 Tue Slivinski, Laura, MS53, 9:30 Wed Slivinski, Laura, MS53, 10:30 Wed Smarslok, Benjamin P., CP17, 3:20 Thu Smith, Lenny, MS19, 5:30 Mon Smith, Ralph C., MS59, 10:30 Wed Smith, Richard, MS24, 5:30 Mon Soane, Ana Maria, CP4, 2:20 Mon Sochala, Pierre, CP13, 9:50 Wed Soize, Christian, MS16, 2:00 Mon Soize, Christian, MS33, 9:30 Tue Solonen, Antti, MS59, 10:00 Wed Somersalo, Erkki, MS50, 4:30 Tue Sousedik, Bedrich, CP4, 3:40 Mon Spantini, Alessio, MS48, 5:00 Tue Spiessl, Sabine M., CP5, 5:50 Mon Spiliopoulos, Konstantinos, MS62, 3:30 Wed Spiller, Elaine, MS90, 2:00 Thu Spiller, Elaine, MS98, 4:30 Thu Spiller, Elaine, MS98, 5:30 Thu Stadler, Georg, MS7, 9:30 Mon Stark, Philip, PD1, 11:30 Tue Stark, Philip, MS42, 5:30 Tue Stefanescu, Elena, MS70, 4:30 Wed Stewart, James R., MS16, 2:00 Mon Stewart, James R., MS16, 2:00 Mon Stewart, James R., MS33, 9:30 Tue Stodden, Victoria, MT4, 2:00 Tue Stodden, Victoria, MT4, 2:00 Tue Stodden, Victoria, MS42, 4:30 Tue Stodden, Victoria, MS42, 4:30 Tue Stoyanov, Miroslav, MS63, 2:30 Wed Stuart, Andrew, IP3, 8:15 Tue Subr, Kartic, MS17, 4:30 Mon Sudret, Bruno, CP10, 2:20 Tue Sullivan, Tim, MS79, 9:30 Thu Sun, Yunwei, MS49, 5:00 Tue Swiler, Laura, MS12, 2:00 Mon Swiler, Laura, MS21, 4:30 Mon Swiler, Laura, MS29, 9:30 Tue Swiler, Laura, MS77, 6:00 Wed

### T

Tan, Matthias H., CP6, 5:50 Mon Tartakovsky, Alexandre, MS91, 2:30 Thu Tartakovsky, Daniel M., MS51, 10:00 Wed Tavakoli, Reza, MS80, 10:30 Thu Teckentrup, Aretha L., MS57, 10:30 Wed Teckentrup, Aretha L., MS69, 5:30 Wed Tempone, Raul F., MS2, 9:30 Mon Tempone, Raul F., MS1, 10:30 Mon Tempone, Raul F., MS19, 4:30 Mon Tempone, Raul F., MS27, 9:30 Tue Tempone, Raul F., MT7, 9:30 Thu Tempone, Raul F., MT7, 9:30 Thu Tenorio, Luis, MS55, 9:30 Wed Tenorio, Luis, MS64, 2:00 Wed Tenorio, Luis, MS64, 3:30 Wed Tenorio, Luis, MS74, 4:30 Wed Tenorio, Luis, MS83, 9:30 Thu Terejanu, Gabriel A., MS55, 9:30 Wed Terejanu, Gabriel A., MS64, 2:00 Wed Terejanu, Gabriel A., MS74, 4:30 Wed Terejanu, Gabriel A., MS83, 9:30 Thu Tesei, Francesco, CP7, 10:10 Tue Thacker, Carlisle, MS71, 6:00 Wed Thakkar, Niket, PP1, 8:00 Mon Tipireddy, Ramakrishna, MS54, 11:00 Wed Tipireddy, Ramakrishna, CP18, 3:40 Thu Tkachenko, Pavlo, PP1, 8:00 Mon Tong, Charles, MS40, 2:00 Tue Tong, Charles, MS49, 4:30 Tue Tong, Charles, MS49, 5:30 Tue Tran, Hoang A., MS57, 11:00 Wed Tuo, Rui, MS84, 9:30 Thu

# U

Ullmann, Elisabeth, MS43, 5:00 Tue

Van Bloemen Waanders, Bart G., MS30, 9:30 Tue Van Bloemen Waanders, Bart G., MS30,

9:30 Tue Van Wyk, Hans-Werner, MS66, 2:00 Wed Van Wyk, Hans-Werner, MS66, 2:00 Wed

Varvia, Petri, MS59, 11:00 Wed Vasylkivska, Veronika S., CP13, 11:10 Wed

Vemaganti, Kumar, CP16, 2:40 Thu Venturi, Daniele, MS6, 9:30 Mon Villa, Umberto E., CP7, 10:30 Tue Vittaldev, Vivek, MS47, 5:00 Tue Vrugt, Jasper, MS71, 5:00 Wed

### W

Wahba, Grace, IP2, 1:00 Mon Wallace, William E., CP8, 10:50 Tue Wan, Xiaoliang, MS65, 2:00 Wed Wang, Chengpu, CP4, 3:20 Mon Wang, Hui, MS56, 10:30 Wed Wang, Junping, PD1, 11:45 Tue Wang, Peng, MS72, 5:00 Wed Wang, Qiqi, MS6, 11:00 Mon Wang, Rui, MS17, 5:00 Mon Wang, Ting, CP5, 4:30 Mon Wang, Weichung, MS25, 4:30 Mon Wang, Xiaochen, MS37, 3:30 Tue Wang, Yan, MS12, 2:00 Mon Wang, Yan, MS21, 4:30 Mon Wang, Yan, MS21, 4:30 Mon Wang, Yan, MS29, 9:30 Tue Watson, Jean-Paul, MS91, 3:00 Thu Weare, Jonathan, MS62, 2:00 Wed Weare, Jonathan, MS72, 4:30 Wed Weare, Jonathan, MS72, 6:00 Wed Webster, Clayton G., MS1, 9:30 Mon

Webster, Clayton G., MS1, 10:00 Mon Webster, Clayton G., MS15, 2:00 Mon Webster, Clayton G., MS18, 4:30 Mon Webster, Clayton G., MS32, 9:30 Tue Webster, Clayton G., MS34, 2:00 Tue Webster, Clayton G., MS43, 4:30 Tue Webster, Clayton G., MS57, 9:30 Wed Webster, Clayton G., MS96, 4:30 Thu Wechsler, Risa, MS85, 6:00 Thu Weiler, Christoph, MS95, 3:00 Thu Weller, Grant B., MS24, 6:00 Mon Wells, Danny, MS20, 5:30 Mon Wildey, Tim, MS87, 10:30 Thu Willcox, Karen E., MS67, 2:00 Wed Willcox, Karen E., MS77, 4:30 Wed Williamson, Danny, MS41, 2:30 Tue Wolpert, Robert L., MS98, 6:00 Thu Woods, David, MS8, 11:00 Mon Wu, Jeff, MS76, 4:30 Wed Wu, Zhen, MS73, 4:30 Wed Wu, Zhen, MS82, 9:30 Thu Wu, Zhen, MS82, 11:00 Thu Wu, Zhen, MS92, 2:00 Thu Wu, Zhen, MS100, 4:30 Thu Wynn, Henry, CP6, 4:30 Mon

Xiong, Jie, MS82, 10:00 Thu Xiu, Dongbin, MS34, 2:30 Tue Xiu, Dongbin, MS51, 9:30 Wed Xiu, Dongbin, MS51, 9:30 Wed Xiu, Dongbin, MS70, 4:30 Wed Xiu, Dongbin, MS79, 9:30 Thu Xiu, Dongbin, MS89, 2:00 Thu Xiu, Dongbin, MS97, 4:30 Thu

Υ

Yadav, Vineet, MS46, 5:00 Tue Yang, Tzu-wei, MS65, 3:30 Wed Yang, Xianjin, MS49, 5:00 Tue Yang, Xiu, MS93, 3:00 Thu Yang, Yahan, MS86, 10:30 Thu Ye, Ming, MS32, 10:30 Tue Yoon, Hongkyu, CP1, 10:30 Mon

### Z

Zabaras, Nicholas, CP9, 3:00 Tue Zabaras, Nicholas, MS97, 4:30 Thu Zahm, Olivier, CP18, 3:20 Thu Zaspel, Peter, MS35, 3:30 Tue Zavala, Victor, MS91, 2:00 Thu Zavala, Victor, MS91, 2:00 Thu Zertuche, Federico, CP10, 3:20 Tue Zhang, Dongxiao, MS16, 3:00 Mon Zhang, Guannan, MS34, 3:00 Tue Zhang, Guannan, MS56, 9:30 Wed Zhang, Guannan, MS57, 9:30 Wed Zhang, Guannan, MS65, 2:00 Wed Zhang, Guannan, MS75, 4:30 Wed Zhang, Guannan, MS73, 4:30 Wed Zhang, Guannan, MS82, 9:30 Thu Zhang, Guannan, MS84, 9:30 Thu Zhang, Guannan, MS92, 2:00 Thu Zhang, Guannan, MS100, 4:30 Thu Zhang, Xuan, MS93, 2:30 Thu Zhao, Weidong, MS73, 4:30 Wed Zhao, Weidong, MS73, 6:00 Wed Zhao, Weidong, MS82, 9:30 Thu Zhao, Weidong, MS92, 2:00 Thu Zhao, Weidong, MS100, 4:30 Thu Zhou, Chao, MS100, 5:00 Thu Zhou, Tao, CP6, 6:10 Mon Zhou, Tao, MS92, 2:30 Thu Zhou, Xiang, MS56, 9:30 Wed Zhou, Xiang, MS65, 2:00 Wed Zhou, Xiang, MS75, 4:30 Wed Zhou, Xiang, MS75, 5:30 Wed Zhou, Xiang, MS84, 9:30 Thu Zhuang, Jiancang, MS90, 3:00 Thu Zunino, Paolo, MS45, 5:00 Tue Zygalakis, Kostas, MS2, 9:30 Mon

# Notes

# UQ14 Budget

# Conference Budget SIAM Conference on Uncertainty Quantification March 31 - April 3, 2014 Savannah, GA

Total\$156,845Expenses*********************************	Expected Paid Attendance	475	
Printing\$3,400Organizing Committee\$4,000Invited Speakers\$11,250Food and Beverage\$22,800AV Equipment and Telecommunication\$18,500Advertising\$4,800Conference Labor (including benefits)\$46,416Other (supplies, staff travel, freight, misc.)\$7,565Administrative\$14,265Accounting/Distribution & Shipping\$7,004Information Systems\$12,525Customer Service\$4,639Marketing\$7,204Office Space (Building)\$3,933Other SIAM Services\$4,459Total\$172,760Net Conference Expense(\$15,915Support Provided by SIAM\$15,915		Total	<u>\$156,845</u> \$156,845
Support Provided by SIAM \$15,915	Printing Organizing Committee Invited Speakers Food and Beverage AV Equipment and Telecommunication Advertising Conference Labor (including benefits) Other (supplies, staff travel, freight, misc.) Administrative Accounting/Distribution & Shipping Information Systems Customer Service Marketing Office Space (Building)	Total	\$3,400 \$4,000 \$11,250 \$22,800 \$18,500 \$4,800 \$46,416 \$7,565 \$14,265 \$14,265 \$7,004 \$12,525 \$4,639 \$7,204 \$3,933 \$4,459 \$172,760
	Net Conference Expense		(\$15,915)
Estimated Support for Travel Awards not included above:			\$15,915 \$0

### Estimated Support for Travel Awards not included above:

Early Career and Students	27	\$19,400
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# Hotel Floor Plan Hyatt Regency Savannah





RIVER STREET

