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.

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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 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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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CP1

Parameter Identification Via Sensitivity and Optimization

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.

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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.

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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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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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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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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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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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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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 ionosphere-thermosphere 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 non-intrusive 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 industrial-scale 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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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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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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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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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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CP4

A New Uncertainty-Bearing Floating-Point Arithmetic

A new deterministic floating-point arithmetic called precision arithmetic is developed to track precision for arith-

metic 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 uncertainty-bearing 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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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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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 process-based 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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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 regularized PD and finite difference methods is $\mathcal{O}(N^{-1/2})$ while that of GT is $\mathcal{O}(N^{1/2})$.

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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 network-based calibration/validation and surrogate-based optimization for model and test selection to perform uncertainty quantification subject to budget constraints.

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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 single-loop 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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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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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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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 standard MLMC method are also presented.

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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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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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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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CP9

Variational Bayesian Approximations for Nonlinear Inverse Problems

Bayesian formulations represent one of the prominent approaches for addressing problems of model calibration. Existing Bayesian methodologies are hampered by the high-dimensionality 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 sparsity-enforcing 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.

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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 trade-off 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 addi-

tional 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 non-smooth 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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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 mechanism-based 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 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.

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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-in-crossflow 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 shared-memory 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.

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CP15

Quasi Monte Carlo Sample Selection for Dependent 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 well-defined 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, ie., 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.

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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, clamped-clamped 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 models for dynamic structural response.

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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 time- and 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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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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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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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^2, 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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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 high-dimensional 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 mean-reversion 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

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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.

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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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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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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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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 under-resolved 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 under-resolved 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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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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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-the-art 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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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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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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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).

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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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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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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 ε-cost over standard Metropolis-Hastings both theoretically and numerically.

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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 Reduced-order 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 $\mathcal{S}_i \subset \mathcal{S}_{i+1}$, where $\mathcal{S}_{i+1}$ is computed from $\mathcal{S}_i$ 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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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.

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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.

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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.

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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.

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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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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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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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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.

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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 two-dimensional 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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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 $u = (u_1, u_2)$, $u_j \in \mathbb{R}^{N_j}$ $(j = 1, 2,\ N_1 + N_2 = N)$ 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.

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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 first-order 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 rainfall-runoff 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 USACM’ 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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MS16

Uq Benchmark Problems for Subsurface Flows

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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 physics-informed 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.

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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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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.

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MS18

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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 high-dimensional 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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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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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 Assimilation

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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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 $rather than requiring it as an input$. PDA is used in forecast mode to make true use of multimodel dynamics via cross-pollination in time. This clarifies the meaning$s$ of uncertainty and the challenges to its quantification in real world forecasting.

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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 low-dimensional 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.

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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

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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 low-dimensional 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

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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 high-throughput 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, ill-conditioned 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 positive-semidefinite. 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.

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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 Ψ. We show conditions on Ψ 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 sparse-grid 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.

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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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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 derivative-free 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.

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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-mass-damper 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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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 data-adaptive 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 one-dimensional 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 non-intrusive 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 angles-only 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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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 high-dimensional 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, discrete-time 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

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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 high-dimensional 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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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.

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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 fractional-order 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 high-dimensional state of a dynamic system with a low-dimensional 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.

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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 non-intrusive 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 Earth-orbiting 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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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 ot 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_2 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 less-expensive 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 SMC^2

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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 high-fidelity 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 time-dependent 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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MS52

Uncertainties in Carefully Constructed Models in Epidemiology

Not available at time of publication.

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MS52
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MS52
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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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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.

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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.

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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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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.

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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.

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MS55

Bayesian Experimental Design in the Presence of Model Error

Calibration and validation of models are inherently data-driven 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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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.

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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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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.

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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 high-order 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.

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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.

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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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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.

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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 cross-validation 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.

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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 multi-model ensembles. Strategies rely on hierarchical Bayesian modeling. I will review a examples with applications to ocean modeling.

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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.

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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 goal-oriented, 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.

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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

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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 coarse-grained models

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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.

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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.

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MS63

Active Subspace Identification in Surrogate Modeling

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.

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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.

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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.

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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 data-gathering 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?

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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.

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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.

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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.

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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

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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.

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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 lower-dimensional 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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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 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.

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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.

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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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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.

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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.

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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.

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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 domain-decomposed 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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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.

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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 least-squares 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.

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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 high-dimensional 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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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 Wales 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.

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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.)

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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.

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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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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.

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MS80

Towards Non-Gaussian Nonlinear Smoothing and 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 steadliy 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 CO2 plume.

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MS81

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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 DRBSDEs 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.

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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 closed–form 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.

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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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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 Applications 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.

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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

Assesing 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 bi-level 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 Lithium-ion 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 curse-of-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 coarse-scale 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 co-simulation 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 Modelling 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 (epidemic-type 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.

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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 day-ahead 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.

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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¿1/2

We obtain a maximum principle for stochastic control problem of general controlled stochastic differential systems driven by fractional Brownian motions (of Hurst index H¿1/2). 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 Feymman-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 spatio-temporal 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 applications, 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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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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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.

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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 high-dimensional joint probability distribution. Hidden variables are naturally introduced to capture the effect of fine scale variables on coarse grained responses. The hyper-parameters 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 relatitvelysimpler. 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 hazard 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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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.

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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.

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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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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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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.

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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.

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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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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 λ 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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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.

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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.

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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.

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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 "matrix-free" 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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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 second-order 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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