IP1

Scalable Algorithms for PDE-Constrained Optimization Under Uncertainty

We consider optimization problems governed by PDEs with infinite dimensional random parameter fields. Such problems arise in numerous applications: optimal design/control of systems with stochastic forcing or uncertain material properties or geometry; inverse problems with stochastic forward problems; or Bayesian optimal experimental design problems with the goal of minimizing the uncertainty or maximizing the information gain in the inferred parameters. Monte Carlo evaluation of the objective as per the popular Sample Average Approximation (SAA) algorithm results in an optimization problem that is constrained by N PDE systems, where N is the number of samples. This results in an optimization problem that is prohibitive to solve, especially when the PDEs are "complex' (large-scale, nonlinear, coupled) and discretization of the infinite-dimensional parameter field results in a high-dimensional parameter space. We discuss high-order derivative-based approximations of the parameter-to-objective maps that, in combination with randomized algorithms, exploit the structure of these maps (smoothness, low effective dimensionality). Their use as a basis for variance reduction is demonstrated to significantly accelerate Monte Carlo sampling and permit solution of problems with $O(10^6)$ uncertain parameters. This work is joint with Peng Chen and Umberto Villa (ICES, UT Austin).

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IP2

On Gradient-Based Optimization: Accelerated, Stochastic and Nonconvex

Many new theoretical challenges have arisen in the area of gradient-based optimization for large-scale statistical data analysis, driven by the needs of applications and the opportunities provided by new hardware and software platforms. I discuss several recent results in this area, focusing on: (1) a new framework for understanding Nesterov acceleration, obtained by taking a continuous-time, Lagrangian/Hamiltonian/symplectic perspective, (2) a discussion of how to escape saddle points efficiently in nonconvex optimization, and (3) the acceleration of Langevin diffusion.

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IP3

A Contemporary View of High-dimensional Quasi Monte Carlo

The numerical computation of expected values as high-dimensional integrals is a central task in uncertainty quantification. Quasi Monte Carlo (QMC) methods are deterministic numerical integration methods that aim for better efficiency (and hence lower cost) than traditional Monte Carlo methods. Originally they were designed with the sole aim of obtaining convergence rates close to $1/N$ (where N is the number of evaluations of the integrand) for smooth enough integrands, compared to the Monte Carlo rate of $1/\sqrt{N}$. But little or no attention was paid to the dependence of the error on s, where s is the number of variables, or the dimension. Nowadays, however, integrals with very large numbers of variables are being tackled, with s in the thousands or tens of thousands or more, and as a result there is as much concern about the dependence on s as on N. The aim of this talk is to present highlights of recent progress on QMC for high-dimensional problems. The highlights include algorithms and software for QMC rules tailored to solutions of elliptic PDE with random coefficients, with error bounds provably independent of the cutoff dimension in this infinite-dimensional problem. In a different direction, there are now high-order QMC rules, rules with potential convergence rates of order $1/N^2$ or even faster.

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IP4

Model Uncertainty and Uncertainty Quantification

The Bayesian paradigm provides a coherent approach for quantifying uncertainty given available data and prior information. Aspects of uncertainty that arise in practice include uncertainty regarding parameters within a model, the choice of model, and propagation of uncertainty in parameters and models for predictions. In this talk I will present Bayesian approaches for addressing model uncertainty given a collection of competing models including model averaging and ensemble methods that potentially use all available models and will highlight computational challenges that arise in implementation of the paradigm.

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IP5

Three Principles of Data Science: Predictability, Stability, and Computability

In this talk, I'd like to discuss the intertwining importance and connections of three principles of data science in the title in data-driven decisions. Making prediction as its central task and embracing computation as its core, machine learning has enabled wide-ranging data-driven successes. Good prediction implicitly assumes stability between past and future. Stability (relative to data and model perturbations) is also a minimum requirement for interpretability and reproducibility of data driven results (cf. Yu, "Stability" in Bernnouli, 2013). It is closely related to uncertainty assessment. The three principles will be demonstrated in the context of two neuroscience projects and through analytical connections. In particular, the first project adds stability to predictive modeling used for reconstruction of movies from fMRI brain signlas to gain interpretability of the predictive model. The second project uses predictive transfer learning that combines AlexNet, GoogleNet and VGG with single V4 neuron data for state-of-the-art prediction performance. It provides stable function characterization of neurons via (manifold) deep dream images from the predictive models in the difficult primate visual cortex V4 and such images are good candidates for follow-up experiments to probe the neurons for confirmation. Our V4 results lend support, to a certain extent, to the resemblance of these CNNs to a primate brain.

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IP6

Multi-level and Multi-index Monte Carlo Methods in Practice

The multilevel Monte Carlo method has proven to be very powerful to compute expectations of output quantities of a stochastic model governed by differential equations. It exploits several discretization levels of the underlying equation to dramatically reduce the overall complexity with respect to a standard Monte Carlo method. However, its practical implementation in complex engineering problems affected by a large number of uncertain parameters still presents considerable challenges. We overview in this talk recent improvements and extensions of the MLMC idea, to include concurrent types of discretization (multi-index Monte Carlo method) and to compute derived quantities such as central moments, quantiles, or cdfs of output quantities. We illustrate then the power of the MLMC method on applications such as compressible aerodynamics, shape optimization under uncertainty, ensemble Kalman filter and data assimilation.

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IP7

Data Assimilation and Uncertainty Quantification A Lagrangian Interacting Particle Perspective

The assimilation of data into computational models and the quantification of forecast uncertainties is central to many application areas including meteorology, hydrology, seismology, power networks etc. Broadly speaking, currently used data assimilation techniques fall into one of the following three categories: (i) variational methods, (ii) Markov chain Monte Carlo methods, and (iii) sequential particle filters. Among sequential particle filters, the ensemble Kalman filter (EnKF) has become very popular but its wider application has been limited by its inherent Gaussian distributional/ linearity assumptions. In my talk, I will focus on recent particle filter extensions of the EnKF to high-dimensional problems with non-Gaussian uncertainties and to combined state-parameter estimation problems. Unifying mathematical principles in these developments are Lagrangian interacting particle representations and optimal coupling arguments.

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IP8

Good and Bad Uncertainty: Consequences in UQ and Design

Engineering decisions are invariably made under substantial uncertainty about current and future system cost and response. However, not all variability is equally detrimental. The possibility of exceptionally high performance can be viewed as good uncertainty, while the chance of failure is usually perceived as bad uncertainty. From this perspective, we examine uncertainty quantification and its use in engineering design. We introduce models for uncertainty quantification and decision making based on superquantile risk (s-risk) that distinguish between good and bad uncertainty, avoid paradoxes, and accrue substantial benefits in risk, reliability, and cost optimization. Leveraging multi-fidelity simulations, we describe methods for predicting s-risk at reduced computational cost for complex systems. Examples from naval architecture, earthquake engineering, and energy management illustrate the framework under both parametric and model uncertainty.

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SP1

SIAG/Uncertainty Quantification Early Career Prize Lecture - Multilevel Markov Chain Monte Carlo Methods for Uncertainty Quantification

Multilevel Monte Carlo methods have become increasingly popular over the last decade, due to their simplicity and their ability to significantly outperform standard Monte Carlo approaches in complex simulation tasks. In this talk, we will discuss how the multilevel methodology can be applied in the context of Markov chain Monte Carlo sampling. The general algorithm will be demonstrated on the particular example of sampling from the posterior distribution in a Bayesian inverse problem, where the goal is to infer the coefficient of an elliptic partial differential equation given observations of the solution. Numerical experiments confirm that the multilevel methodology reduces the computational effort to achieve a given tolerance by several orders of magnitude.

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CP1

Probabilistic Graphical Model Based Approach for Nonlinear Stochastic Dynamic Analysis

Uncertainty quantification in dynamical systems is often difficult due to the high dimensionality of the system responses and inputs as well as the non-linear nature of the underlying model. The proposed approach attempts to mitigate these issues. It utilizes a probabilistic graphical model (PGM) framework together with a Gaussian process (GP) surrogate model and expectation propagation (EP) for performing inference tasks. A factor graph is utilized to efficiently represent the dependencies of the inputs and the response. Latent variables are introduced into the graphical model for tackling dependencies in an efficient manner. Sparse GPs are used to represent the functional relation between the nodes in the factor graph. To learn the parameters associated with the PGM, sequential Monte Carlo, coupled with stochastic gradient descent algorithm is used. Finally, UQ of nonlinear dynamical system is performed by employing EP, which is an efficient approximate Bayesian inference algorithm. Two high-dimensional nonlinear dynamic problems are presented to illustrate the accuracy and efficiency of the proposed framework.

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CP1

Uncertainty Quantification for Numerical Models with Two or More Solutions

Some numerical models have two or more distinct solutions. These can include tipping points and bifurcations, many being discontinuous across the separate solutions. Illustrations include climate systems (eg overturning circulation) and biological systems (eg networks to model the human brain). For example, a computer model may fail to complete in specific regions and we would like to be able to predict where to avoid running the model. We consider how to identify these regions using a latent variable modelled as a Gaussian process (GP). This latent variable acts as an unobserved quantity to help identify the boundary between regions, where initially just 2 output solutions are considered. Given only minimal information from a set of initial inputs and their associated output, each input value is given a corresponding class label; negative for solution 1 and positive for solution 2. The latent GP is estimated using this limited information, and a threshold (normally zero) defines the boundary. Methods explored for estimating the latent GP include the EM algorithm, ABC and MCMC sampling. Results are similar, although MCMC proves to be the most efficient. Extensions to higher dimensions and multiple solutions are discussed. We also consider experimental design aspects, such as the optimum place to add data points to improve estimation of the region boundary. We examine whether it is better to place points to improve the boundary estimate or gain knowledge of the actual system.

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CP1

Gibbs Reference Posterior for Robust Gaussian Process Emulation

We propose an objective posterior distribution on correlation kernel parameters for Simple Kriging models in the spirit of reference posteriors. Because it is proper and defined through its conditional densities, it lends itself well to Gibbs sampling, thus making the full-Bayesian procedure tractable. Numerical examples show it has near-optimal frequentist performance in terms of prediction interval coverage.

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CP1

Uncertainty Quantification of Atmospheric Chemical Transport Models using Gaussian Process Emulators

Atmospheric chemical transport models (CTMs) simulate the production, loss and transport of hundreds of gases in the atmosphere and are used to make local, regional and global forecasts of air quality. There is an urgent need to: (i) understand why CTMs differ significantly in their predictions of important gases such as tropospheric O3, OH and CH4, and (ii) quantify the uncertainty in these predictions. We address these problems by using global sensitivity analysis, model calibration and uncertainty analysis. We are the first to apply these statistical methods across multiple CTMs. These methods require thousands of model runs and so we replace the CTM, which typically takes 12 hours to do a one year run, with a Gaussian process emulator. In this presentation, I will show results to a sensitivity analysis, a model calibration and an uncertainty analysis involving five CTMs, 30 parameters, and model outputs consisting of global maps of O3, CO, and CH4 lifetime. A preliminary analysis found that the differences in predicted global CH4 lifetime by two CTMs is due to predicted CH4 lifetime being sensitive to two different processes, a result which was unexpected. In a separate preliminary analysis which used measurements of O3 and CO and a MCMC routine, we reduced the uncertainty of the parameters that had the largest influence on the O3 and CO outputs of a CTM. This had the knock-on effect of reducing the uncertainty in the modelled predictions of O3 and CO.

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CP1

Nonstationary Gaussian Process Emulation of Computer Models via Cluster-based Covariance Mixtures

A common assumption, adopted when constructing a Gaussian Process emulator, is the stationarity of the covariance function, implying a global smoothness for the simulator response. However, stationary Gaussian Process emulators perform poorly for simulators, that exhibit heterogeneity and local features. Stationary Gaussian Processes become overconfident in high variability regions of parameter space and underconfident in regions where the simu-

lator is well-behaved. We propose a new method of constructing nonstationary Gaussian Process emulators based on a spatial covariance structure proposed by Banerjee et al. (2004). We identify L distinct regions across the input space found from clustering standardized errors from an initial stationary fit and for each region we define its own covariance function with the corresponding parameters. The covariance function of the nonstationary GP emulator is a sum of the L covariance functions with the mixture parameters derived from the Bayesian clustering. We examine the performance of our method against stationary Gaussian Process emulator, Treed Gaussian Process model (TGP) [Gramacy and Lee, 2008] and Composite Gaussian Process model (CGP) [Ba and Joseph, 2012] on a number of numerical examples. The application of our nonstationary method to the modelling of boundary-layer potential temperature for convection in the CNRM climate model [Voldoire et al., 2011] is provided.

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CP2

Reduced Order Model for Random Vibroacoustic Problems

The robust design of vibroacoustic systems requires a taking into account of possibly numerous sources of uncertainties in the model in order to predict their impact on the response. It reveals necessary to develop reliable and efficient tools for the prediction of such responses and in this framework, functional approaches for uncertainty quantification suffer from the highly nonlinear behaviour of the response to the input uncertainties. In order to tackle such problems, we consider statistical learning methods based on least squares minimization for high d-dimensional problems where the output is approximated in suitable low-rank tensor formats. The storage complexity of these formats grows linearly with the dimension d which makes possible the construction of an approximation using only few samples. However the rank of the approximation of the stochastic dynamic response may be high and the method thus loses its efficiency. The key is to proposea suitable functional representation and an adapted parametrization with $M < d$ variables for the computation of the response so to obtain structured approximations with low complexity. The latter parametrization is determined automatically by coupling a projection pursuit method and low rank approximation.

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CP2

Progressively Refining Reduced Order Models for Estimating Failure Probabilities of Dynamical Systems

Reduced order models (ROMs) help to accelerate simulations of dynamical systems. Therefore they are being increasingly used for estimating failure probabilities. However, the use of ROMs yields erroneous estimates, primarily due to (i) approximation error from size reduction, and (ii) training error. The training error may arise from suboptimal selection of training points or inaccurate interpolation of ROMs. To address these issues, a new algorithm is proposed here that refines ROMs progressively, thereby attempting to minimize both errors. Accordingly, the ROM size is gradually increased to reduce the error from approximation, while retaining computational efficiency. Further, the training domain of the ROMs is progressively localized to reduce the error from training. The algorithm is robust with respect to the choice of model reduction method and training. It can also be easily parallelized as it is based on a statistical simulation. The proposed algorithm is used to estimate the failure probability of a bridge structure under the action of a moving inertial mass. The uncertainty is assumed to be in the material modulus of elasticity. ROMs are developed using proper orthogonal decomposition, and interpolated on the tangent space to a Grassmann manifold. The algorithm is shown to be able to estimate failure probabilities with sufficient accuracy while offering significant computational gain.

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CP2

Stochastic Analysis and Robust Optimization of a Reduced Order Model for Flow Control

This contribution targets a probabilistic robustness and sensitivity analysis for the validation and robust amelioration of a Reduced Order Model (ROM) that was deduced from a High Fidelity Model (HFM) simulating the flow field around a high-lift configuration airfoil. The ROM is to be used for closed-loop flow control by means of Coandă blowing. For the robustness analysis a general Polynomial Chaos Expansion (gPCE) based surrogate model was used. In the probabilistic framework, the ROM becomes a stochastic ODE with random coefficients, where both the state of the flow and the coefficients are approximated with a general polynomial chaos expansion (gPCE). This gPCE is also used for an efficient global sensitivity analysis to investigate the influence of variation of the coefficients on the uncertainties of the state of the flow. Besides checking the robustness of the model, the objective here is to gain more information about the influence of the individual modes and to validate the confidence region of the derived model on the solution of the ROM by evaluating variance based global sensitivities. This information can facilitate the decision making on the number of the needed modes and amelioration of the model by further tuning the ROM coefficients by Bayesian inversion. This inverse method is carried out such way to preserve as much of the underlying physics of the High Fidelity Model and its model structure as much possible.

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CP2

Reduced Order Modeling for Nonlinear Structural Analysis using Gaussian Process Regression

A non-intrusive reduced basis (RB) method is proposed for parameterized nonlinear structural analysis considering large deformations and elasto-plastic constitutive relations. In this method, a reduced basis is constituted from a set of full-order solutions employing the proper orthogonal decomposition (POD), then Gaussian process regression (GPR) is used to approximate the projection coefficients onto the reduced space. The GPR is carried out in the offline stage with the aid of active data selection by a greedy algorithm, and the outputs for different parameters can be rapidly obtained as probabilistic distributions in the online stage. Due to the complete decoupling of offline and online stages, the proposed RB method provides a powerful tool to efficiently solve the parameterized nonlinear problems with various engineering applications such as structural optimization, risk analysis, real-time evaluation and parameter identification. With both geometric and material nonlinearities taken into account, numerical results are presented for some typical 1D and 2D examples, illustrating the accuracy and efficiency of the proposed method.

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CP2

Probabilistic Model Validation of Large-scale Systems using Reduced Order Models

Multiple mathematical models are often available to describe a physical system. Identifying which of those models are useful to represent the physical system is essential to making engineering decisions. In this study, a probabilistic framework is used, where models that cannot reasonably describe the measurements are first falsified by controlling an error criterion, namely false discovery rate (FDR). Among the remaining model classes, appropriate models and/or model class(es) are then chosen using a model selection algorithm. Finally, the quality of the selected model class(es) is rechecked. To alleviate the computational burden of such validation exercises for large-scale systems it proposed herein to use reduced order models (ROMs). A ROM for each model class is first constructed and trained over the entire parameter domain for the falsification step and then adaptively trained for the model selection step. The proposed approach is illustrated using an 11-story 99-degree-of-freedom building where different model classes are formed by considering different flexural rigidities at different stories combined with different levels of support constraints. The ROMs are constructed using proper orthogonal decomposition. The use of the proposed framework is shown to give significant computational savings proportional to those offered by the ROMs.

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CP2

Quantifying Uncertainty in Reduced Models for Discrete Fracture Networks

Reduced modeling is becoming increasingly necessary to yielding fast results for complicated, expensive models. Although many models rely on a similar modeling methodology for reduction, ie taking a matrix system and reducing it while maintaining of the same properties as the larger system, there are other avenues. A large-scale computational model for transport was developed at Los Alamos National Laboratory that uses discretized meshes for the forward solution. A reduced model was created using graph networks to simplify the problem. We propose to model the uncertainty in quantities of interest, such as pressure, by using the graph model. We propose to test our uncertainties against well-established results of the high-fidelity model as proof of trust for use in larger and unknown transport problems.

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CP3

Random Partial Differential Equations on Moving Hypersurfaces

Although partial differential equations with random coefficients (random PDEs) is very popular and developed field, it seems that the analysis and numerical analysis of parabolic random PDEs on surface still appears to be in its infancy. Surface PDEs appear in many applications such as image processing, cell biology, porous media etc. Uncertainty of parameters naturally appears in all these models, which motivates us to combine these two frameworks: geometry of domain and uncertainty. In this talk we will first consider analysis of random advection-diffusion equation on evolving hypersurfaces. After introducing appropriate setting for this problem that combines geometry and probability, we will prove its well-posednees in appropriate Sobolev-Bochner space. Both, uniform and log-normal diffusion coefficient will be considered. Furthermore, we will introduce and analyse a surface finite element discretisation of the equation. We will show unique solvability of the resulting semi-discrete problem and prove optimal error bounds for the semi- discrete solution and Monte Carlo samplings of its expectation. Our theoretical findings are illustrated by numerical experiments in two and three space

dimensions.

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CP3

Uncertainty Quantification of PDEs on Random Domains using Hierarchical Matrices

We are interested in the first and second moment of the solution of PDEs with random input data. Previous works have shown that these moments can be computed by the hierarchical matrix arithmetics in almost linear time if the solution depends linearly on the data. However, in the case of random domains the dependence of the solution of the data is nonlinear. Extending previous perturbation approaches we can linearize the problem and can compute the first and second moment up to third order accuracy in almost linear time.

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CP3

UQ for Nearly Incompressible Linear Elasticity

This talk presents some recent developments in error estimation associate with robust formulations of linear elasticity. Our focus is on uncertainty quantification. We discuss stochastic Galerkin finite element (SGFEM) approximation of two alternative mixed formulations of linear elasticity with random material parameters. Specific numerical results confirm the validity of our theoretical results.

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CP3

Domain Decomposition Solvers for Spectral Sfem Versus Non-intrusive Sparse Grid Based Solvers for Large Stochastic Dimensions

A three-level scalable domain decomposition (DD) algorithm which employs an efficient preconditioner at each level is developed to solve the coarse system in the Galerkin projection based intrusive spectral finite element method. The numerical and parallel scalabilities of this solver are first studied for a stochastic PDE with non-Gaussian system parameters represented as a stochastic process using up to 25 random variables. The computational efficiency of the intrusive DD solver is then demonstrated over sparse grid base non-intrusive method.

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CP3

Optimal Iterative Solvers for Linear Systems with Random PDE Origins: 'Balanced Black-box Stopping Tests'

This talk will discuss the design and implementation of efficient solution algorithms for symmetric indefinite and nonsymmetric linear systems associated with FEM approximation of PDE problems (Stokes and Navier–Stokes equations in particular) with random coefficients. The novel feature of our preconditioned MINRES and GMRES solvers is the incorporation of error control in the 'natural' norm in combination with a reliable and efficient a posteriori estimator for the PDE approximation error. This leads to a robust and optimally efficient stopping criterion: the iteration is terminated as soon as the algebraic error is insignificant compared to the approximation error. A stopping criterion for the (nonlinear) Newton solver is also presented.

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CP3

Advection-Diffusion PDEs with Random Discontinuous Coefficients

Advection-diffusion equations arise in various applications, for instance in the modeling of subsurface flows. We consider this type of partial differential equations with random coefficients, which may then account for insufficient measurements or uncertain material procurement. To represent, for example, transitions in heterogeneous media, we include spatial discontinuities in the parameters of the equation. For a given temporal discretization, we solve a second order elliptic problem in each time step where the random coefficient is given by the sum of a (continuous) Gaussian random field and a (discontinuous) jump part. By combining multilevel Monte Carlo sampling techniques and pathwise finite element methods we are able to estimate moments of the solution to the random partial differential equation. To stabilize the numerical approximation and accelerate convergence, we introduce an adaptive, pathwise triangulation for the finite element approximation which accounts for the varying discontinuities in each sample of the coefficients. This is joint work with Andrea Barth (SimTech, University of Stuttgart)

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CP4

Parameter Identification for a Viscoplastic Model with Damage and Effect of Conditions on Results using Bayesian Approaches

The state of materials and accordingly the properties of structures are changing over the period of use, which may influence the reliability and quality of the structure during its life-time. Therefore identification of the model parameters and states of the system is a topic which has attracted attention in the content of structural health monitoring.
In this work the focus is on identification of material parameters and states of a viscoplastic damaging material. It is proposed to use Bayesian inverse methods for this. To do so, two steps are considered, solving the forward and inverse problem. Therefore, first the propagation of the a priori parametric uncertainty through the model including damage describing the behaviour of a steel structure is studied. A non-intrusive Stochastic Finite Element Method (SFEM) based on polynomial chaos is applied. From the forward model, material parameters and interval unobservable state variables can be identified using measurement data such as displacement via Bayesian approaches. In this study, two methods are applied. The first is a Polynomial chaos based update method which is a modification of Kalman filter and the second one is a transitional Markov chain Monte Carlo method. At the end, the results of both methods are compared.
We study the effect of load conditions and sensor placements, which provide us the observation, on the identification procedure and how much information they provide to the identification process.

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CP4

Parameter Calibration and Model Validation of JWL Equation of State Based on Multi-output

The adjustable parameters in JWL equation of state need to be calibrated to match the detonation simulation results and experimental data. However, no model is perfect. The model bias in physical models may have a significant impact on the results of parameter calibration. The cross-validation based on multi-output is one of the effective methods to identify model bias. The cylinder test is the benchmark experiment to evaluate output energy of the explosive and calibrate parameters of JWL equation of state for explosive products. The traditional calibration method is usually only based on radius data in the radial direction. As the improvement of test technology, both the radius and velocity can be observed in cylinder test. In this paper, we propose that the Gaussian process and wavelet methods are used to build surrogate models for the radius and velocity respectively. Then three statistical models are considered for calibration, that is both radius and velocity, only radius, only velocity. At last three calibration results are used for model validation.

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CP4

Bayesian Inference for Estimating Model Discrepancy of an Electric Drive Model

The exponential increase of available compute power allows to leverage the potential of uncertainty quantification (UQ) in new applications assuming an industrial setup. A main challenge is related to the fact that the considered models are rarely able to represent the true physics and demonstrate a discrepancy compared to measurement data. Further, an accurate knowledge of considered model parameters is usually not available. E.g. fluctuations in manufacturing processes of hardware components introduce uncertainties which must be quantified in an appropriate way. This requires efficient methods for UQ based on Bayesian inference. An important task related to Bayesian inference is to accurately estimate parameter distributions from measurement data in presence of simulation model inadequacy.

As a first step, we address this challenge by investigating the influence of model discrepancies onto the calibration of model parameters and further consider a Bayesian inference framework including an attempt to correct for model discrepancy by an additional term. Synthetic measurement data from an industrial application is then used to evaluate the framework. First measurement data is created with an electric drive model and second another electric drive model containing an artificial model discrepancy is used to infer physical parameters and the model discrepancy term. The application shows a promising perspective of the framework by good approximation of discrepancy and parameters.

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CP4

Stochastic Reconstruction of Porous Media from Voxel Data

We describe a novel method to generate computer models of an aluminum foam given its CT-data, such that the generated samples are similar to the target foam in terms of the statistics of a selection of microstructural descriptors. The generated samples could later be used in flow simulations in order to investigate the relationships between the material's effective properties, such as permeability, conductivity, etc., and its microstructure.
Currently used methods to generate such samples are either very time-intensive or inaccurate (in terms of being unable to match important microstructural descriptors). In order to address this issue, a novel stochastic model based on the generalised ellipsoid equation has been devised, which when incorporated into a Markov chain Monte Carlo framework, is capable of producing structures that are statistically close to the target structure within a reasonable time frame. In this presentation, the aforementioned model and the framework will be described along with an analysis of the quality of the reconstructed samples.

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CP4

Characterizing Errors and Uncertainties in Non-equilibrium Molecular Dynamics Simulations of Phonon Transport

Non-equilibrium molecular dynamics (MD) is commonly used for predicting phonon transport and estimating thermal conductivity of material systems. A heat flux is imposed along a specific direction and the resulting steady state temperature gradient is used to estimate the thermal conductivity based on Fourier's law. This methodology however is known to exhibit large discrepancies from experimental measurements of bulk thermal conductivity. In this work, we study the impact of size and input heat flux on such discrepancies for silicon using the Stillinger-Weber (SW) inter-atomic potential. Since thermal conductivity estimates are based on the nominal values of the SW potential parameters, we investigate variability in these estimates by perturbing the individual parameter values. Furthermore, we perform sensitivity analysis and calibrate important parameters in a Bayesian setting using the available experimental data. Non-intrusive polynomial chaos surrogates are employed to overcome computational hurdles associated with sensitivity analysis as well as Bayesian calibration. However, since construction of PC surrogates itself can be expensive, we demonstrate methodologies that exploit derivate-based sensitivity measures [Kucherenko et al., 2009], and active subspaces [Constantine, 2015] to reduce the dimensionality of the problem.

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CP4

Challenge of Detonation Modeling in Extreme Condition and its Uncertainty Quantification Methods

The mathematical and physical model of Solid explosive is described by coupling nonlinear partial differential equations. First of all, the mathematical model of the solid explosive detonation is nonlinear partial differential equations in extreme condition. Much uncertainty exists in this empirical model. Second, solid explosive detonation is a complex dynamical problem with multi-layer, multi-scale such as microcosmic, macroscopic, and microscopic process. Third, in the real numerical prediction process, we first search for optimal value the confidence interval of random (uncertain) variable based on the standard experiment calibration and uncertain optimization. Then the result is used for prediction. The computation volume of classical approach is huge due to wide range of the search space and loss of structure information. We must deal with the computational expense and large scale computing problems in order to get the expected efficiency and stability. Fourth, it is difficult to establish appropriate model to exactly describe this process when considering these uncertainty. It is also a challenge. Base on the above discussion, this paper analyze the weakness and strength of current uncertainty quantification methods, then propose a Bayesian parameter calibration method of JWL equation of state in explo-

sive detonation based on the surrogate model.

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CP5

Uncertainty Quantification of Locally Nonlinear Dynamical Systems using Polynomial Chaos Expansion

The problem of uncertainty propagation for a nonlinear dynamical system involves specifying the statistics or the probability distribution of the quantities of interest. However, propagating this uncertainty becomes computationally burdensome for large-scale complex nonlinear systems. An important class among these large-scale systems are those with spatially-localized nonlinearities. In this study, a computationally efficient algorithm is proposed using a generalized polynomial chaos expansion while reducing the order of the system using a nonlinear Volterra integral equation for locally-nonlinear dynamical systems. A fast Fourier transform significantly reduces the computational effort of solving the resulting low-order Volterra integral equations. An adaptive procedure for dividing the random parameter space for the expansions is also introduced here to further enhance the efficiency of the proposed algorithm. The proposed approach is used to estimate the mean and variance of the roof acceleration of a 100 degree-of-freedom building model with a localized nonlinearity in the base isolation layer, which is modeled using a Bouc-Wen hysteresis model. This building is subjected to a historic earthquake excitation. The proposed algorithm shows great computational efficiency achieved compared to standard uncertainty quantification methods.

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CP5

Uncertainty Quantification for an Optical Grating Coupler using Adaptive Stochastic Collocation

Due to the progress in nanotechnological manufacturing, photonic components can nowadays be designed by structures which are even smaller than the optical wavelength. These optical devices are a promising technology, e.g., plasmonic structures show great potential for guiding and controlling light. Numerical simulations play an important role in the design process of such devices. A challenging problem is that input data is not exactly known, due to manufacturing imperfections which have a significant impact on nanoscale devices. Therefore, statistical information about S-parameters of such stochastic systems based on statistical information about the uncertain input data is of great interest. In this work we quantify uncertainties in the finite element model of a plasmon waveguide [Preiner et al, Efficient optical coupling into metal-insulator-metal plasmon modes with subwavelength diffraction gratings, APL, 2008]. The considered structure is periodic in two dimensions and therefore the computational domain can be confined to a single unit cell on which Maxwell's source problem is solved. In order to cope with a large number of uncertain and very sensitive parameters an adaptive sparse grid algorithm is applied [Schieche, Unsteady Adaptive Stochastic Collocation Methods on Sparse Grids, PhD thesis, 2012].

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CP5

Estimation of Plume Dispersion in Hetrogeneous Formations by Transformed Adaptive Stochastic Collocation Method

The plume dispersion of contaminants in hetrogeneous formations is dominated by spatial variability of flow velocities associated with the hydraulic conductivities. In general, the solute statistics can be calculated by the Monte Carlo simulations, in which multiple realizations of a plume are generated. The drawback of the Monte Carlo method is that it usually requires a large number of realizations and could be computationally prohibitive. Instead, the stochastic collocation method, based on sparse grids, serves as an alternative approach. However, estimation of plume dispersion using the stochastic collocation method has two challenges. First, when the correlation length is small compared to the space domain, there will be a large number of random dimensions after KarhunenLove decomposition, then the number of collocation points will increases dramatically, i.e., curse of dimensionality. Second, the solute concentration has an unsmooth profile when the dispersivity is small, hence the convergence rate of the stochastic collocation method could be rather slow. In this study, a transformed adaptive stochastic collocation method is proposed, which adaptively selects the important random dimensions and introduce an additional stage to transform the unsmooth concentration to smooth arrival time. The proposed method is tested in two- and three-dimensional examples with different spatial variances and correlation

lengths to illustrate its accuracy and efficiency.

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CP5

Adaptive Sparse Interpolation Methods for Electromagnetic Field Computation with Random Input Data

In many applications of science and engineering, time- or resource-demanding simulation models are often substituted by inexpensive polynomial surrogates in order to enable computationally challenging tasks, e.g. optimization or uncertainty quantification studies of field models. For such approaches, the surrogate model's accuracy is of critical importance. Moreover, in the case of many input parameters, the curse-of-dimensionality substantially hampers the surrogate's construction. State-of-the-art methods employ interpolation on adaptively constructed sparse grids, typically based on Clenshaw-Curtis [B. Schieche, *Unsteady Adaptive Stochastic Collocation Methods on Sparse Grids*, TU Darmstadt, 2012] or, more recently, Leja [A. Narayan and J.D. Jakeman, *Adaptive Leja Sparse Grid Constructions for Stochastic Collocation and High-Dimensional Approximation*, SIAM J. Sci. Comput., 2014] nodes. These methods provide accurate surrogate models, mitigating or altogether avoiding the curse-of-dimensionality, at the cost of a relatively small number of unused original model evaluations. In this work, we shall use a benchmark example from the field of computational electromagnetics in order to compare the aforementioned methods with respect to computational cost and accuracy. Moreover, we will suggest enhancement approaches, aiming to reduce the costs caused by unused model evaluations during the surrogate model's construction.

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CP5

Adaptive Pseudo-spectral Projection for Time-dependent Problems

Polynomial Chaos Expansions (PCEs) are popular spectral surrogate models typically applied to solve uncertainty propagation problems. They are used to quantify the effect of statistical fluctuations in simulation model outputs due to uncertainty in parameter space. Various techniques exist to compute the coefficients of PCEs. A canonical way is to approximate the coefficients by numerical quadrature, evaluate the simulation model at the quadrature nodes and post-process the results. However, this approach suffers from aliasing errors, which can be circumvented by tailoring the PCE to the numerical quadrature (in our case a "Smolyak sparse grid") in a special way. This gives rise to the so-called "Pseudo-Spectral Projection method (PSP)", which can be extended to a dimension adaptive version (aPSP). For time-dependent problems, however, the associated error estimators must take into account variations of errors in time. Depending on the time interval of interest, uncertainties in parameters contribute differently to the overall uncertainty fluctuations of the simulation model outputs. In this talk, we give a short overview on aPSP and investigate the choice of different error estimators for a time-dependent problem with uncertain parameters. The simulation model represents a direct current model for an electrical motor. The focus is on convergence of the error estimators in comparison to "root mean-square errors" obtained by a set of test simulation data.

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CP6

Advanced Sensitivity Analysis for Offshore Wind Cost Modelling

The solution of managerial problems often involves the creation of dedicated decision support models, which are complex and potentially involve inputs subject to uncertainty, meaning that the resulting relationships between inputs and outputs are poorly understood. This is the case for the Offshore Wind Cost Analysis Tool (OWCAT) developed at the EDF Energy R&D UK Centre; given the increased complexity, modellers can no longer grasp the response of the model outputs to variations in inputs based solely on intuition. As a result, three global sensitivity analysis methods have been considered for OWCAT: Morris, Sobol variance-based and PAWN density-based. Special attention has been paid to the work of Saltelli, where the most effective Morris or Sobol estimator is chosen based on the sample size. In addition, where variance is not a good proxy for uncertainty, the PAWN technique allows the modeller to identify cases where the uncertainty is misrepresented. A sensitivity analysis toolbox has been created and benchmarked against a set of well-studied test functions, before being applied to OWCAT. The contribution of this talk is to demonstrate the application of these advanced sensitivity analysis techniques not only to theoretical test functions but also to a real-world decision-making case in the offshore wind industry. Useful insight into the model is gained by factor prioritization and factor fixing.

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CP6

The Space of Shapes and Sensitivity Analysis: An Application of Differential Geometry

Engineering designers routinely manipulate shapes in engineering systems toward design goals formulated as a functional over the shape—e.g., shape optimization. Differential geometry provides a set of analytical tools for defining a shape calculus. In particular, we investigate applications using the set of equivalence classes resulting from an S^1 embedding in R^2 given the set of all re-parameterizations. Combining the presented space of shapes with a Soblev-type metric and corresponding shape sensitivity analysis enables the study of a local subspace of shapes on a Riemannian manifold. We discuss a numerical interpretation to estimate important directions in this subspace which change a functional the most, on average.

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CP6

Bayesian Estimation of Probabilistic Sensitivity Measures for Computer Experiments

Simulation-based experiments have become increasingly important for risk evaluation and decision-making in a broad range of applications, in engineering, science and public policy. In the presence of uncertainty regarding the phenomenon under study, in particular, of the simulation model inputs, a probabilistic approach to sensitivity analysis becomes crucial. A number of global sensitivity measures have been proposed in the literature, together with estimation methods designed to work at relatively low computational costs. First in line is the one-sample or given-data approach which relies on adequate partitions of the input space. We propose a Bayesian alternative for the estimation of several sensitivity measures which shows a good performance on synthetic examples, especially for small sample sizes. Furthermore, we propose the use of a nonparametric approach for conditional density estimation which bypasses the need for pre-defined partitions, allowing the sharing of information across the entire input space through the underlying assumption of partial exchangeability. In both cases, the Bayesian paradigm ensures the quantification of the uncertainty in the estimation.

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CP6

Efficient Evaluation of Reliability-oriented Sensitivity Indices

The role of simulation has kept increasing for the analysis of complex systems. In that prospect, global sensitivity analysis studies how the uncertainty in the code output can be apportioned to the uncertainty in the different stochastic code inputs. However, most of the classical sensitivity methods, such as the Sobol indices, focus on the central tendency of the output. When interested in the analysis of undesirable events associated with small probabilities, such sensitivity indices may thus be not meaningful. This motivated the proposal of reliability-oriented sensitivity indices. However, the evaluation of these indices generally requires a huge number of dedicated code evaluations, which can lead to extremely high total computational cost. To circumvent this problem, the present work proposes a method to evaluate several kinds of reliability-oriented sensitivity indices, which is only based on the code evaluations that were needed to compute the probability of occurrence of the considered undesirable event. After having introduced the theoretical basis of this method, several applications will be presented to illustrate its efficiency.

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CP7

Using Computer Models and UQ to Diagnose Diastolic Heart Failure

Diastolic heart failure is a currently untreatable condition that is caused by stiffness of the heart. We investigate the possibility of diagnosing the condition using data from MRI scans, a numerical model of the heart, simulating a single beat, and uncertainty quantification. To invert the model we use history matching. This involves building an emulator so that we can predict the model results (with associated uncertainty) at any point in input space and hence an implausibility score. Those parts of input space that are implausible are ruled out. Running further waves of model runs within the not implausible region reduces it until this region is not reduced any further or becomes zero. The model is then calibrated. If there are no not implausible points we have to adjust the model discrepancy how well we expect the model to reproduce the data. To carry this out we need to make a number of choices. We need to reduce the dimension of the problem (the initial dimension is high) without losing vital information. There are regions of input space where the modelled heart is too stiff to beat and so the model run does not complete. We do not want to emulate these regions so we find a way of predicting where they are. We also discuss model discrepancy. This is a measure of how well we expect the model to perform for the chosen metric and is an integral part of history matching. We show that not-implausible regions for healthy and sick patients are disjoint.

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CP7

Fluid-structure Interaction with Uncertainty in Medical Engineering

In recent decades biomedical studies with living probands (in vivo) and artificial experiments (in vitro) have been complemented more and more by computation and simulation (in silico). In silico techniques for medical diagnosis can give enhanced information for the risk stratification of cardiovascular surgery. Making surgical decisions, high reliability is a requirement for diagnostic methods. Since uncertainties are inherent to the measurement-based simulation input data, a quantification of their impact is needed for reliability analysis. For cardiovascular applications, such as the simulation of blood flow through the aorta, the physiological understanding and modeling has still challenging aspects with respect to the uncertainty. We present a numerical framework for the three-dimensional simulation of aortic blood flow with elastic vessel wall movement including uncertainty quantification. The underlying fluid-structure interaction (FSI) problem is calibrated patient-specifically by magnetic resonance imaging. The resolution of the vessel geometry as well as of the time profile of the measured flow is limited up to a certain accuracy. Furthermore, the non-invasive measurement of the stiffness of the aortic vessel wall is highly challenging. This leads to uncertainties in the physical parameters of the underlying mathematical model. We present an approach to efficiently compute patient-specific aortic FSI simulations incorporating UQ based on high performance computing.

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CP7

Bayesian Uncertainty Quantification for Epidemic Spread on Networks

While there exist a number of mathematical approaches to modeling the spread of disease on a network, analyzing such systems in the presence of uncertainty introduces significant complexity. In scenarios where system parameters must be inferred from limited observations, general approaches to uncertainty quantification can generate approximate distributions of the unknown parameters, but these methods often become computationally expensive if the underlying disease model is complex. In this talk, I will apply Π4U, a recent massively parallelizable Bayesian uncertainty quantification framework, to a model of disease spreading on a network of communities, showing that the method accurately and tractably recovers system parameters and selects optimal models in this setting.

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CP7

Data-extraction Uncertainty in Meta-analysis of Published Medical Data

The data required for meta-analysis are often not available for extraction in published medical studies (for example, the true number of deaths). Often these data are missing due to loss-to-follow up. It may be possible to infer the missing data using other information available in the papers, such as Kaplan Meier survival plots. If the probability of survival is extracted, an estimated number of deaths could be inferred and a meta-analysis computed. However, the survival probability is an estimate with associated uncertainty. Current meta-analysis models do not account for the uncertainty associated with the data estimations and may result in potentially inaccurate conclusions. We propose methods to model the uncertainty that occurs at the data-extraction step and properly propagate it into the final meta-analysis estimates.

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CP7

Uncertainty Quantification for the Reliable Simulation of a Blood Pump Device

Heart failure (HF) is a severe cardiovascular disease, it happens when the heart muscle is so weakened such that it can not provide sufficient blood as body needs. More than 23 million people are suffered by HF worldwide. Despite the modern transplant operation is well established, the lack of heart donations becomes a big restriction on transplantation frequency. Therefore, ventricular assist devices (VADs) can play an important role in supporting patients during waiting period and after the surgery. We consider an intrusive Galerkin projection based on the generalized Polynomial Chaos (gPC). The intrusive Galerkin approach can represent stochastic process directly at once with Polynomial Chaos series expansions, and therefore optimizes the total computing effort comparing with classical non-intrusive methods. We compared different preconditioning techniques for a steady state simulation of a blood pump configuration in our previous work, the comparison shows that an inexact multilevel preconditioner has a promising performance. In this work, we show an instationary blood flow through a Food Drug Administration blood pump configuration with Galerkin Projection method, which is im-

plemented in our open source Finite Element library Hiflow3. Three uncertainty sources are considered: inflow boundary condition, rotor angular speed and dynamic viscosity, the numerical results are demonstrated with more than 40 Million degrees of freedom by using supercomputer.

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CP8

High Performance Computing for Uncertainty Quantification: Challenges and Perspectives for Flow Problems

The available compute power on high performance computers (HPC) is still increasing exponentially. This tremendous increase of capacity in the last decade is mainly due to the growth of the number of cores used for a given numerical simulation. Beside scalability and data locality issues taking full advantage of intrinsic features remains a challenging task, even for pure deterministic models. Typical setups for which this issues may become highly critical can be found e.g. in computational fluid mechanics (CFD). Such problems are usually modeled by the Navier-Stokes equations, which include parameters which can not always be assumed to be known accurately. Taking such uncertainties into account by stochastic models results in a parametrization by a set of independent random variables. This leads to a blown up system size requiring even more scalable numerical schemes in order to take advantage of the capabilities of high performance computers. This talk discusses the impact of emerging hardware technology in HPC for uncertainty quantification (UQ) applied to CFD. The link between contemporary deterministic approach and intrusive schemes based on stochastic Galerkin methods using Polynomial Chaos will be established. A simplified performance model based on the computational intensity is presented and allows to evaluate the quality and the efficiency of UQ approaches in the context of CFD. Numerical experiments assuming complex flow problems are presented.

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CP8

Eigenspace-based Uncertainty Characterization in Large-Eddy Simulation of Turbulent Flow

Large-Eddy Simulation (LES) has gained significant importance as a high-fidelity technique for the numerical resolution of complex turbulent flow. In comparison to Direct Numerical Simulation (DNS), LES approaches reduce the computational cost of solving turbulent flow by removing small-scale information from the conservation equations via low-pass filtering. However, the effects of the small scales on the resolved flow field are not negligible, and therefore their contribution in the form of Sub-Filter Stresses (SFS) needs to be modeled. As a consequence, the assumptions introduced in the closure formulations result in potential sources of structural uncertainty that can affect the Quantities of Interest (QoI). Moreover, unlike DNS, the resolved fluctuations at a size just larger than the "filter width" still have significant energy. This complicates the control of numerical errors which become important sources of numerical uncertainty that can impact the QoIs both directly through the resolved scales and indirectly via the modeled SFS. The aim of this work is to characterize the importance of these two types of uncertainty and their impact on the QoIs by means of recently developed eigenspace-based strategies that decompose the SFS tensor in magnitude, shape and orientation, to facilitate the analysis. In the presentation, the strategy will be described in detail and results from LES of turbulent flow will be discussed.

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CP8

Predictive Simulations for Calculating Wind Loads on Buildings

Computational fluid dynamics can be used in wind engineering applications to quantify pressure loads on buildings and assess wind hazards, but simulations of atmospheric boundary layer flows are strongly influenced by uncertainty in the inflow boundary condition and the turbulence model. In the present work we quantify the uncertainty in a Reynolds-averaged Navier-Stokes simulation of a wind tunnel experiment of a high-rise building. The objective is to predict the mean pressure coefficient distribution on the lateral building facade with a quantified confidence interval, and to compare the results to the experimental data. The uncertainty in the inflow condition is characterized using 3 uncertain parameters (reference velocity, roughness length and model orientation), and then propagated to the quantities of interest using a polynomial chaos expansion approach. The results indicate that the uncertainty in the inflow conditions is non negligible, but insufficient to explain the discrepancy with the wind tunnel test data. We subsequently investigate the uncertainty related to the turbulence model, using a framework that introduces perturbations in the Reynolds stress tensor. The performance of this method is evaluated by comparing the results to a large-eddy simulation of the same building configuration. The results demonstrate some shortcomings in the existing approach, and indicate that a multi-fidelity simulation framework might be required to achieve the objective.

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CP8

Estimation of Uncertainty of Turbulence Model Predictions in SU2

Reliable predictions for turbulent flows are of fundamental importance for a variety of engineering analysis and design applications. Herein, Reynolds-Averaged Navier Stokes models represent the workhorse for industrial design and investigations. Owing to the closure assumptions utilized in their formulation, RANS models introduce a significant measure of model-form uncertainty in the predictions. The estimation and eventually, reduction of these uncertainties is of great interest to ensure that turbulent models can be reliable predictive tools in industrial analysis and design. Many methodologies to estimate this uncertainty are currently being developed. However, these are typically implemented only in proprietary codes. A vast majority of industrial simulations involving turbulent flows utilize commercial or open-source CFD codes. At present, such turbulence model-form uncertainty estimation is not available on any such software suite. We implement and demonstrate the Eigenspace Perturbation framework for turbulence model-form uncertainty estimation in the SU2 CFD suite. SU2 is an open-source compressible analysis and design framework that utilizes unstructured mesh technology to represent complex geometric shapes typical of industrial practice. This implementation is tested over a series of turbulent flows, benchmark test cases and flows of engineering import, and the computed uncertainty bounds are contrasted against experimental data & high-fidelity simulations.

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CP8

Validation of a Framework for Data Assimilation and Uncertainty Quantification for Urban Flow Predictions

The numerical prediction of urban wind flows is fundamental to ensure the design of resilient and sustainable cities. For example, computational fluid dynamics results can help to optimize pedestrian wind comfort, air quality, natural ventilation strategies, and the deployment of wind turbines. However, the significant variability and uncertainty associated with the atmospheric boundary layer poses an important challenge to the accuracy of the results. To understand the effect of uncertainties in the models and develop better predictive tools, we started a pilot study that combines a numerical analysis with a field measurement campaign on Stanford Universitys campus. We consider the incoming wind direction and magnitude as uncertain parameters and perform a set of Reynolds-averaged Navier-Stokes simulations to build a polynomial chaos expansion response surface at each sensor location. We subsequently assimilate the measurement data from strategically deployed sensors, using an inverse ensemble Kalman filter to iteratively infer the probability distributions for the inflow parameters. Once these distributions are obtained, the forward analysis is repeated to obtain predictions for the flow field in the entire urban canopy and the results are compared with the experimental data from several other wind sensors. This procedure enables a better characterisation of the uncertainty in the results and improves the confidence in our wind flow predictions.

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CP9

Global Optimization of Expensive Functions using Adaptive Radial Basis Functions Based Surrogate Model via Uncertainty Quantification

Global optimization of expensive functions has important applications in physical and computer experiments. It is a challenging problem to develop efficient optimization scheme, because each function evaluation can be costly and the derivative information of the function is often not available. We propose a novel global optimization framework using adaptive Radial Basis Functions (RBF) based surrogate model via uncertainty quantification. The framework consists of two iteration steps. It first employs an RBF-based Bayesian surrogate model to approximate the true function, where the parameters of the RBFs can be adaptively estimated and updated each time a new point is explored. Then it utilizes a model-guided selection criterion to identify a new point from a candidate set for function evaluation. The selection criterion incorporates the expected improvement (EI) of function prediction and its uncertainties. We conduct simulation studies with standard test functions to show that the proposed method is more efficient and stable in searching the global optimizer compared with a prominent existing method.

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CP9

Solving Stochastic Optimal Power Flow Problem via Polynomial Chaos Expansions

Uncertainty quantification has recently become of significant importance in the field of power systems. This development originates, among others, from the huge influx of renewable energy sources to the power grid. The natu-

ral fluctuations of wind/solar energy call for a structured consideration of uncertainties such that a reliable supply of electrical energy can be provided in the future. The so-called optimal power flow (OPF) problem is a cornerstone in the operational planning of power systems. The goal of this nonconvex optimization problem is to determine operating points for power systems such that a (monetary) cost is minimized while technical limitations (e.g. generation limits, line flow limits) and the nonconvex power flow restrictions are respected. The talk will discuss how the OPF problem formulation and solution change in the presence of stochastic uncertainties, leading to stochastic OPF. Starting from existing approaches we will show that polynomial chaos expansion allows a unified framework to formulate and solve stochastic OPF problems in the presence of (non)Gaussian uncertainties. Polynomial chaos allows to answer affirmatively what generation policies are optimal, i.e. how the power generation is adjusted optimally in the presence of stochastic uncertainties. We will support our findings by IEEE test case simulations implemented in Julia. To this end, first steps towards a Julia package for generalized polynomial chaos are presented as a byproduct.

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CP9

Topology Optimization using Conditional Value at Risk

Traditional approaches to formulating stochastic topology optimization problems for additive manufacturing tend to use linear combinations of the mean and standard deviation of a design figure of merit (e.g., compliance). However, this choice of objective/constraint underweights tail events for non-normal random variables. We propose replacing these mean-plus-standard-deviation expressions with the conditional value-at-risk (CVaR), and argue that it better compensates for worst-case tail events.

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CP9

Uncertainty Quantification for Stochastic Approximation Limits using Chaos Expansion

We investigate the analysis of uncertainty quantification of the limit of a stochastic approximation (SA for short) algorithm. Typically, this limit $\phi^\star$ is the zero of a function h written as an expectation of H; this naturally arises in various problems about optimization, statistics, control etc. In our study, the limit $\phi^\star$ is subjected to uncertainty through a parameter θ (related to the probabilistic model used for the expectation or to the definition of H), and we aim at deriving the probabilistic distribution of $\phi^\star(\theta)$ as θ has a distribution π. Our approach consists in decomposing $\phi^\star$ on a $L^2(\pi)$-orthogonal basis (Chaos Expansion), and in computing the basis coefficients using a suitable dimension-increasing SA algorithm. Under mild assumptions, we prove the almost-sure convergence of this SA algorithm in the underlying infinite-dimensional Hilbert space. Numerical results support our theoretical analysis. Notably, the possibility of letting the number of estimated expansion coefficients tend to infinity appears not only as a necessary ingredient for proving the theoretical convergence of the algorithm, but also as a key feature from a numerical performance point of view, including for the estimation of the lower order coefficients.

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CP10

A Bayesian Approach for Quantifying the Uncertainty of Physical Models Integrated into Computer Codes

We adopt a Bayesian approach to address an inverse problem arising in uncertainty quantification. The issue is to assess the uncertainty of physical models integrated into computer codes by means of indirect physical measurements. To do so, a non-intrusive approach is followed in this work where the code is taken as a "black-box" function. After introducing a statistical model that links the available physical measurements to the corresponding code outputs, a Gibbs sampler based on the full conditional distributions is laid out in both linear and non linear settings. However, as the computer simulations are moderately expensive, it tends to become impractical in reasonable time. To overcome this difficulty, we propose to replace the computer code with a Gaussian process emulator which can deliver both robust and quick predictions of the code outputs. An industrial application to a thermal-hydraulic code at the system scale is displayed where the uncertainty of two condensation models for safety injections is assessed.

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CP10

When Models and Data Disagree: Sparse Resolutions to Inconsistent Datasets in B2BDC

Bound-to-Bound Data Collaboration (B2BDC) provides a deterministic optimization-based framework for Uncertainty Quantification. In this approach, parameters are constrained by combining both polynomial surrogate models and experimental observations with interval uncertainty. A collection of such models and observations is termed a dataset and carves out a feasible region in the parameter space. If the models and data agree within uncertainty, then this feasible set is non-empty and the dataset is consistent. In real-world application, however, it is often the case that diverse collections of experiments and observations are inconsistent. Revealing the source of this inconsistency, i.e., identifying which models and/or obser-

vations are problematic, is essential. In this presentation, we discuss a constraint relaxation-based approach, entitled the vector consistency measure, for investigating datasets with numerous sources of inconsistency. This tool seeks a sparse set of relaxations by minimizing an L1-penalty. The benefits of this vector consistency approach over a previous method of consistency analysis are demonstrated in two realistic gas combustion examples.

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CP10

Beyond Black-boxes in Model-based Bayesian Inverse Problems

Two of the most important roadblocks in the solution of model-based Bayesian inverse problems are: a) the curse of dimensionality, b) the difficulty in quantifying structural, model errors. We propose a novel framework which recasts the solution of PDEs encountered in continuum thermodynamics as probabilistic inference over function spaces. This formulation foregoes the expensive solution of a forward or adjoint problem by considering all physical state variables as latent, random variables constrained by the governing equations of the forward model. It also provides an alternative approach for solving inverse problems, since it defines a unified, probabilistic view where both the differential operator as well as the observations represent sources of information that is incorporated into the final posterior. In contrast to traditional, black-box approaches, the probabilistic modeling and resolution of individual state variables allows to quantify inadequacies of the model in a physically interpretable manner and to assess their effect in the solution.

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CP10

4D-Var Data Assimilation using Exponential Integrators

We consider four-dimensional variational (4D-Var) data assimilation problems for evolutionary differential equations. For the time discretization, exponential propagation iterative methods of Runge-Kutta type (EPIRK) are used, which can achieve a high order of accuracy and are well suited for stiff problems. Based on (noisy) measurements, given at different points in time, we maximize the posterior using gradient based optimization in combination with a discrete adjoint approach. We use a W-method, which allows model independent approximations of the Jacobian while preserving the accuracy of the scheme. Additionally, the occurrence of Hessian matrices in the adjoint problem can be avoided. The discrete adjoint code itself is obtained using algorithmic differentiation. Two application examples will be considered for illustration: we will use 4D-Var to estimate the initial conditions of the Lorenz-96 model and discuss a computational magnetics problem, where the unknown parameters characterize the nonlinearity of the magnetic material.

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CP10

Bayesian Inversion for High Dimensional Systems using Data Assimilation

A poor estimation of model parameters is one of the main sources of uncertainty in any physical system. Over the years, different data assimilation methods have been implemented to acquire improved estimations of model parameters. They correct the uncertain parameters by assimilating the observed data based on the likelihood function of Bayesian framework in such a way that the mathematical model approximates the true state as closely and consistently as possible. However, most of these methods are either developed on the assumption of Gaussian pdfs or have the limitation of high computational expenses. Thus there is a high demand of new more efficient methods. In this research work, we propose a generic sequential Monte Carlo (SMC) approach as a combination of ensemble transform particle filter and tempering. Ensemble transform particle filter is a data assimilation technique developed on the backbone of Bayesian approach with the framework of linear transport problem. While tempering ensures a smoother transition from the prior distribution to posterior distribution. We implement a twin experiment based on Darcy flow model to examine the performance of this new approach with other SMC methods. The numerical experiments demonstrate that in physical systems with non-Gaussian distributions the proposed method is more efficient in accurately capturing the multi-modal posterior distribution.

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CP10

Inverse Problem for Random-parameter Dynami-

cal Systems

The problem of estimation of parameters of a dynamical system from discrete data can be formulated as the problem of inverting the map from the parameters of the system to points along a corresponding trajectory. Presented will be an overview of recent results in this area, specifically, (i) conditions for identifiability of linear and linear-in-parameter systems from a single trajectory, (ii) analytical and numerical estimates of the maximal permissible uncertainty in the data for which the qualitative features of the inverse problem solution for linear systems (such as existence, uniqueness, or attractor properties) persist, and (iii) techniques for identification of deterministic processes with uncertain parameters from distribution of data.

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CP11

Self-Exciting Point Processes and Uncertainty Quantification in Recording and Forecasting Long Duration Episodic Phenomena Like Volcanic Events

Several sources of uncertainty affect our knowledge of the past eruptive record in every volcanic system. Unknown sub-sequences of past eruptions with ill-constrained dating are common, and sometimes the under-recording issues may be substantial. Clustering phenomena are often observed in the data, violating any simplifying assumption of memorylessness. Moreover, the necessity of gathering a sufficiently large dataset of past events often implies going far into the past, and hence dealing with the progressive evolution of the volcanic system. Frequency, size, chemistry and location of activity can greatly change in the long term. We present the modeling choices that we made in case studies of Campi Flegrei caldera (Italy), and Long Valley volcanic region (CA, USA) to deal with these problems. We use a Cox process to enable uncertainty quantification in the outputs. We test alternative self-exciting and non-stationary assumptions to compensate for system evolution, without discarding the older, but still useful information. In particular: (i) forward simulation of the processes allows for their self-development, and can flexibly adapt to the observed history without needing an arbitrary prescription of trends or additional long-lasting information structures; (ii) the processes fit well to the most recently observed data, but they also use the entire past history to calibrate their evolving features.

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CP11

Bayesian Inference on Uncertain Kinetic Parameters for the Pyrolysis of Composite Ablators

The heat shield of high speed reentry spacecraft is often made up of porous ablative thermal protection materials (TPMs) that can accommodate high heating rates and heat loads through phase change and mass loss. When the temperature increases, those materials absorb heat and start to pyrolyze, releasing gases that interact with the surrounding flow. Modeling the species production and the material decomposition rate is important for their use in numerical simulations for the robust determination of heat shield thickness. To this end, pyrolysis experiments have been performed on TPMs in order to determine the kinetic parameters of chemical laws that govern mass loss and species production rates [Wong et al., Polym. Degrad. Stabil., 112:122131, 2015]. Samples are heated in a furnace and the mass loss is measured while the species produced are collected. In this talk, we introduce the context of physico-chemical modeling of ablation, the experiments, and the sources of uncertainty. We present the model used to link the kinetic parameters to the experimental observations by means of Arrhenius laws. We then state the formulation of the inverse problem in a Bayesian framework and we discuss the elaboration of an appropriate likelihood function. We finally present results of the inversion procedure, with particular attention to the influence of the number of species taken into account in the model.

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CP11

Bayesian Updating for Uncertain Condition State using Monitoring and Sequential Inspections

Structural Health Monitoring using permanent sensors has been a fast growing management tool during the last decade. This is mostly due to technological advances in

This progress resulted in decreasing cost and improving efficiency. However, till this date, the installation of sensors on every measurable feature of the structure stills prohibitory costly. As such one must rely on the measures of a few judiciously placed sensors to predict the condition states of the structure elements. The low number of sensors induces various types of uncertainties related to measurement techniques and structural behavior. In this paper, the uncertain condition states of the structural members are considered in the integrity assessment. An approach is proposed for a Bayesian updating of the condition states, based on the output of the monitoring sensors. The posterior probability distribution describing the magnitude of the defect for each element is further updated by inspecting a few elements in an optimal sequence such that the posterior probability distribution for the remaining not inspected elements reaches an optimal threshold of likelihood about their condition states. A numerical application of the proposed methodology is presented. A sensitivity analysis is performed for the optimal cost with respect to various parameters such as sensor configuration, inspection result uncertainty, etc., in order to highlight the potential benefits of the proposed approach.

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CP11

A Bayesian Coarse-graining Approach to the Solution of Stochastic Partial Differential Equations

Well-established methods for the solution of stochastic partial differential equations (SPDEs) such as stochastic collocation methods or polynomial chaos expansions typically struggle with high dimensionality of the stochastic space. Moreover, finite element approximations to the forward model require discretizations small enough to resolve the variability of the underlying random fields, leading to a large and expensive set of algebraic equations. We introduce a data-driven, physically-inspired probabilistic surrogate modeling approach which combines Bayesian coarse-graining of the involved random fields with multi-fidelity techniques that allow accurate reconstruction of the fine scale response given the repeated, but much cheaper evaluation of the PDE on a coarser discretization. By automatically detecting and retaining only features of the stochastic process which are most predictive to trace back the fine scale solution, we are able to work in the regime of high dimensional uncertainties (thousands) but only few forward model runs (tens). The model achieves sublinear complexity and is fully probabilistic, i.e. we obtain predictive distributions that accurately quantify both model and limited data uncertainties. The proposed approach is validated with different problems in random media.

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CP11

Bayesian Model Averaging Kriging

Metamodels are widely used to approximate the response of computationally-intensive engineering simulations for a variety of applications. They are formulated based on an observation of the original numerical model. Among the variety of metamodeling techniques, Kriging has gained significant popularity. Kriging models the underlying input/output function by combining two parts: a regression model that expresses the global mean behavior, and a zero-mean stationary Gaussian Process (GP) that captures localized deviations from the global one. Conventional Kriging approaches construct the regression model with a single set of basis functions. Selection between different candidate sets of basis functions is typically deterministically performed, choosing a single model based on some optimality criterion. In this contribution, a Bayesian model class averaging formulation is adopted to consider different sets of basis functions in establishing the Kriging predictions. Each of these models is weighted by its respective posterior model probability when aggregating the final predictions. To enable the computationally efficient application, a data-driven and tractable prior distribution is proposed, and multiple strategies in the inference and prediction stage are presented. Numerical examples show that the proposed Kriging implementation is capable of constructing a more accurate metamodel than other alternatives with comparable computational cost.

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CP11

Climate Model Discrepancy: Thinking Outside of the UQ Toolbox

The Uncertainty Quantification community has widely accepted the need to quantify and include model discrepancy when estimating the parameters of complex physical models. Due to well-known identifiability problems with traditional Bayesian approaches, structured prior knowledge is required for model discrepancy in order to reach appropriate parameter estimates. Climate models represent a special challenge for existing UQ methods. Climate model calibration (what the community calls tuning), if done the traditional Kennedy-OHagan way, would require structured prior specification for discrepancy over many of the massive spatio-temporal fields that make up the terabytes of output produced by climate models and satellite/station observations. We will argue that the way these models are constructed makes the specification of well informed structured discrepancy judgements over these fields infeasible. We present a delayed-Bayesian approach to parameter inference that involves first verifying the models capability to simulate emergent climate processes, then using the results of this analysis for structured prior discrepancy modeling and a formal calibration to complete tuning. These ideas

will be presented in the form of a case study working with the Canadian climate model CanAGCM4.

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CP12

Nonparametric Functional Calibration of Computer Models

Standard methods in computer model calibration treat the calibration parameters as constant throughout the domain of control inputs. In many applications, systematic variation may cause the best values for the calibration parameters to change between different settings. When not accounted for in the code, this variation can make the computer model inadequate. We propose a framework for modeling the calibration parameters as functions of the control inputs to account for a computer model's incomplete system representation in this regard while simultaneously allowing for possible constraints imposed by prior expert opinion. We demonstrate how inappropriate modeling assumptions can mislead a researcher into thinking a calibrated model is in need of an empirical discrepancy term when it is only needed to allow for functional dependence of the calibration parameters on the inputs. We apply our approach to plastic deformation of a visco-plastic self-consistent material in which the critical resolved shear stress is known to vary with temperature.

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CP12

The Interacting Particle System Method Adapted to Piecewise Deterministic Processes

The reliability assessment of complex power generation systems generally relies on simulation methods. When the system failure is a rare event, the MC methods are computationally intensive and we need to use a variance reduction method to accelerate the reliability assessment of such system. Among variance reduction methods, one may think of particles filters methods such as the interacting particle system method (IPS). This method is well suited to industrial applications, because it does not require much knowledge about the system.
Such power generation systems often follow deterministic dynamics which can be altered by isolated components' failures, components' repairs, or automatic control mechanisms. In order to model these dynamic hybrid systems, we use piecewise deterministic Markovian processes. When simulated on a short period of time, such processes tend to often generate the same deterministic trajectory, thus limiting the efficiency of the IPS method for which it is preferable to generate many different trajectories on short intervals of time. To reduce this phenomenon, we propose an adaptation of the IPS method based on the memorization method: conditioning the generated trajectories to avoid the most probable ones while computing exactly the influence of the most probable trajectories. Our adaptation of the SMC method yields an strongly consistent estimator of the reliability, which has the advantage of having a smaller asymptotic variance.

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CP12

Approximate Optimal Designs for Multivariate Polynomial Regression

We introduce a new approach aiming at computing approximate optimal designs for multivariate polynomial regressions on compact (semi-algebraic) design spaces. We use the moment-sum- of-squares hierarchy of semidefinite programming problems to solve numerically the approximate optimal design problem. The geometry of the design is recovered via semidefinite programming duality theory. This work shows that the hierarchy converges to the approximate optimal design as the order of the hierarchy increases. Furthermore, we provide a dual certificate ensuring finite convergence of the hierarchy and showing that the approximate optimal design can be computed with our method. As a byproduct, we revisit the equivalence theorem of the experimental design theory: it is linked to the Christoffel polynomial and it characterizes finite convergence of the moment-sum-of-square hierarchies.

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CP12

Probabilistic Models and Sampling on Manifolds

We present a new approach for sampling probability models supported on a manifold. The manifold is characterized through its manifold diffusion subspace, the probability model is constructed using kernel density estimation and sampling is carried out using a Ito equation projected on the manifold. The procedure serves a number of objectives that are ubiquitous in uncertainty quantification. First, by acknowledging an intrinsic structure discovered from numerically generated simulations, their scatter associated with parametric variations is considerably smaller than viewed in an ambient space. Fewer may thus be required to achieve similar statistical precision. This capability is even more significant for OUU problems where the stochastic simulator is integrated into an optimization loop. We demonstrate this capability on high-dimensional UQ problems with very expensive forward simulators. Second, the projected Ito provides an accurate probabilistic

surrogate for large high-dimensional datasets.

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CP12

Experiment Design in Non-linear Regression with Additional Random Parameters

It is supposed that sequentially in time a variable is measured with random errors. This variable depends on several explanatory variables as well as on a position of a sensor and the relationship is non-linear. Moreover, the regression function contains some additional parameters that are random but their distribution is known. The goal of statistical inference is to find an optimal position of a sensor for estimating parameters of interest. As we may look at the same problem from different perspectives, the optimal designs may differ substantially.

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CP12

Quantifying Uncertainties with Distribution Element Trees

The estimation of probability densities based on data is important in many applications such as for example in the development of Bayes classifiers in supervised learning. In this work, we present a new type of density estimator [D.W. Meyer, Statistics and Computing, 2017, doi:10.1007/s11222-017-9751-9] that is highly adaptive and based on distribution element trees (DET). The DET estimator is particularly advantageous when dealing with large samples and/or samples of high dimensionality. In a range of applications we demonstrate the high accuracy and superior performance in comparison to existing state-of-the-art density estimators such as adaptive kernel density estimation or Polya and density tree methods. Finally, we point out the possibility of using DETs as an elegant means for conditional random number generation or smooth bootstrapping.

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CP13

Statistical Learning in Tree-based Tensor Format

Tensor methods are widely used tools for the approximation of high dimensional functions. Such problems are encountered in uncertainty quantification and statistical learning. The high dimensionality imposes to use specific techniques, such as rank-structured approximations. In this lecture, we present a statistical learning algorithm for the approximation in tree-based tensor format which are tensor networks whose graphs are dimension partition trees. This tensor format includes the Tucker format, the Tensor-Train format, as well as the more general Hierarchical tensor formats. It can be interpreted as a deep neural networks with a particular architecture. The proposed algorithm uses random evaluations of the function to provide a tree-based tensor approximation, with adaptation of the underlying approximation spaces, of the tree-based rank and of the dimension partition tree, based on statistical estimates of the approximation error. The method is illustrated on different examples.

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CP13

Low-rank Dynamic Mode Decomposition: Optimal Solution in Polynomial-time

This work studies linear low-rank approximations of high-dimensional dynamical systems using dynamic mode decomposition (DMD). Searching a low-rank approximation can be formalised as attempting to solve a non-convex optimisation problem. However, state-of-the-art algorithms only provide sub-optimal solutions to this problem. This work shows that there exists a closed-form optimal solution, which can be computed in polynomial-time, and gives a characterisation of the ℓ_2-norm of the approximation error. The theoretical results serve to design low-complexity algorithms building low-rank approximations by SVD of the optimal solution or low-rank DMD. The algorithms performance is analysed by numerical simulations using synthetic and physical data benchmarks.

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CP13

Contrast Enhancement in Electrical Impedance Tomography using the Approximation Error Approach

We consider electrical impedance tomography (EIT) imaging of the brain. The brain is surrounded by the poorly conducting skull, which causes a partial shielding effect leading to weak sensitivity for the imaging of the brain tissue. We propose a statistical learning based approach to enhance the contrast in brain imaging. With this approach, the conductivity of the target is modelled as a combination of two unknowns, spatially distributed background and the shielding (skull) layer. The model discrepancy between the forward model with and without the unknown shielding layer is treated as a modelling error noise in the observation model, and then the uncertainty related to the modelling error noise is handled by using the Bayesian approximation error approach. With this approach, the image re-

construction consist of recovering the spatially distributed background conductivity and a low rank approximation of the modelling error, which is then used for estimating an approximation for the unknown shielding layer. The approach is evaluated with simulations and phantom data.

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CP13

A Weighted Reduced Basis Method for Parabolic PDEs with Random Data

We consider the reduced basis method applied to a parametrized, linear parabolic PDE with random input. Statistics of outputs of interest are estimated with the Monte Carlo (MC) method. In order to speed up the computation, the reduced basis method approximates the solution manifold on a low-dimensional subspace, which is constructed by the *POD-greedy* procedure using rigorous error estimators.
The focus of this study is to improve the reduced space construction regarding the expected solution and expected output error using the idea of a weighted *POD-greedy* method. As a reference, a weighted *POD* is used. It builds up an optimal reduced space that minimizes the energy norm of the error in a mean square sense. A comparison between the non-weighted and weighted approach is drawn.

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CP13

Active-subspace Analysis of Up-crossing Probability for Shallow-water Model

A major challenge in marine engineering simulations is to quantify the interdependence of the uncertainties in the input and output model parameters. We consider this interdependence for stochastic ocean waves in a shallow-water wave propagation model, with uncertainties in the kinematic boundary condition (BC). The BC involves 302 random variables that, together with a JONSWAP wave spectrum, define the nonlinear wave surface elevation. We discretize the wave propagation model using generalized Polynomial Chaos (gPC) and a Sparse-Grid non-intrusive Stochastic Collocation Method. Initially, the number of sparse grid points is infeasibly high, and it is therefore reduced using an active-subspace analysis (ASA) [Paul G. Constantine, Active Subspaces Emerging Ideas for Dimension Reduction in Parameter Studies, Society for Industrial and Applied Mathematics, 2015], where important general directions in the parameter space are identified. We then compute the four first statistical moments of the wave surface elevation, and use them in a moment-based Gauss transformation to analyze the up-crossing probability for the shallow-water model. We demonstrate the advantages and the effectiveness of the ASA-gPC approach against classical Monte Carlo implementations.

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CP14

Universal Prediction Distribution

The use of surrogate models instead of computationally expensive simulation codes is very convenient in engineering. Roughly speaking, there are two kinds of surrogate models: the deterministic and the probabilistic ones. These last are generally based on Gaussian assumptions. The main advantage of probabilistic approach is that it provides a measure of uncertainty associated with the surrogate model in the whole space. This uncertainty is an efficient tool to construct strategies for various problems such as prediction enhancement, optimization or inversion. Away from the Gaussian case, many surrogate models are also available and useful. Nevertheless, they are not all naturally embeddable in some stochastic frame. Hence, they do not provide naturally any prediction error distribution. We propose a universal method to define a measure of uncertainty suitable for any surrogate model: deterministic, probabilistic and ensembles. It relies on Cross-Validation sub-models predictions. This empirical distribution may be computed in much more general frames than the Gaussian one. It allows the definition of many sampling criteria. We give and study adaptive sampling techniques for global refinement, inversion and an extension of the so-called Efficient Global Optimization algorithm applicable for all types of surrogate models. The performances of these new algorithms are studied both on toys models and on an engineering design problem.

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CP14

Emulating Dynamic Non-linear Simulators using Gaussian Processes

In this paper, we examine the emulation of non-linear deterministic computer models where the output is a time series, possibly multivariate. Such computer models simulate the evolution of some real-world phenomena over time, for example models of the climate or the functioning of the human brain. The models we are interested in are highly non-linear and exhibit tipping points, bifurcations and chaotic behaviour. Each simulation run is too time-consuming to perform nave uncertainty quantification. We therefore build emulators using Gaussian processes to model the output of the code. We use the Gaussian process to predict one-step ahead in an iterative way over the whole time series. We consider a number of ways to propagate uncertainty through the time series including both the uncertainty of inputs to the emulators at time t and the correlation between them. The methodology is illustrated with a number of examples. These include the highly non-linear dynamical systems described by the Lorenz and Van der Pol equations. In both cases we will show that we not only have very good predictive performance but also have measures of uncertainty that reflect what is known about predictability in each system.

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CP14

Finite-dimensional Gaussian Approximation with Linear Inequality Constraints

Gaussian processes (GPs) is one of the most famous non-parametric Bayesian frameworks for modelling stochastic processes. Introducing inequality constraints in GP models can lead to more realistic uncertainty quantifications in learning a great variety of real-world problems. However, existing GP frameworks either cannot satisfy constraints everywhere in the output space, or are restricted to specific types of inequality conditions. Covariance parameter estimation is also a challenge when inequalities are considered. To the best of our knowledge, the finite-dimensional approach from Maatouk and Bay (2017) is the only Gaussian framework that can satisfy inequality conditions everywhere (either boundedness, monotonicity or convexity). However, their proposed framework still presents some limitations to be improved. Our contributions are threefold. First, we extend their approach to deal with general sets of linear inequalities. We wrote the posterior distribution given the interpolation and inequality constraints as a truncated multivariate Gaussian distribution. Second, we explore several Markov Chain Monte Carlo techniques to approximate the posterior. Third, we investigate theoretical properties of the constrained likelihood for covariance parameter estimation. According to experiments on both artificial and real data, our full framework together with a Hamiltonian Monte Carlo-based sampler provides efficient results on both data fitting and uncertainty quantification.

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CP14

Surrogate Modeling of Two Nested Codes with Functional Outputs

Gaussian process surrogate models are widely used to emulate computationally costly computer codes. In this work we are interested in the case of two nested computer codes, whose outputs are functional. By nested computer codes, we mean that the functional output of the first code is an input of the second code. By working on the structure of the covariance functions, we propose a computationally efficient surrogate model of the functional output of the second code as a function of all the inputs of the nested computer code.

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CP14

Experimental Design for Non-parametric Correction of Misspecified Dynamical Models

We consider a class of misspecified dynamical models where the governing term is only approximately known. Under the assumption that observations of the system's evolution are accessible for various initial conditions, our goal is to infer a non-parametric correction to the misspecified driving term such as to faithfully represent the system dynamics and devise system evolution predictions for unobserved initial conditions. We model the unknown correction term as a Gaussian Process and analyze the problem of efficient experimental design to find an optimal correction term under constraints such as a limited experimental budget. We suggest a novel formulation for experimental design for this Gaussian Process and show that approxi-

mately optimal (up to a constant factor) designs may be efficiently derived by utilizing results from the literature on submodular optimization. Our numerical experiments exemplify the effectiveness of these techniques.

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CP15

Multi-Index Quasi-Monte Carlo and H-Matrices

We consider a new method to generate normal or log-normal random fields from [Feischl et al., 2017+] which builds on fast matrix-vector multiplication via H-matrices. The method proves to be robust with respect to the covariance length of the random field, and is particularly efficient for very smooth and very rough random fields. Moreover, the method applies to a fairly general class of covariance functions and is not limited to the stationary case. We use this new method in combination with quasi-Monte Carlo integration, to solve a Poisson equation with random coefficient. Moreover, to exploit the inherent sparsity of the approximation, and to obtain an efficient algorithm, we use the Multi-Index quasi-Monte Carlo approach in three coordinate directions: the finite-element approximation error, the approximation error of the random field, and the integration error of the quasi-Monte Carlo rule. This allows us to significantly reduce the computational time

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CP15

Stochastic Least-Squares Petrov-Galerkin Method for Parameterized Linear Systems

We consider the numerical solution of parameterized linear systems where the system matrix, the solution, and the right-hand side are parameterized by a set of uncertain input parameters. We explore spectral methods in which the solutions are approximated in a chosen finite-dimensional subspace. It has been shown that the stochastic Galerkin projection technique fails to minimize any measure of the solution error. As a remedy for this, we propose a novel stochastic least-squares Petrov–Galerkin (LSPG) method. The proposed method is optimal in the sense that it produces the solution that minimizes a weighted ℓ^2-norm of the residual over all solutions in a given finite-dimensional subspace. Moreover, the method can be adapted to minimize the solution error in different weighted ℓ^2-norms by simply applying a weighting function within the least-squares formulation. In addition, a goal-oriented seminorm induced by an output quantity of interest can be minimized by defining a weighting function as a linear functional of the solution. We establish optimality and error bounds for the proposed method, and extensive numerical experiments show that the weighted LSPG methods outperforms other spectral methods in minimizing corresponding target weighted norms.

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CP15

A Provably Stable Coupling of Numerical Integration and Stochastic Galerkin Projection

In many real world applications, the uncertainties are not uniformly distributed throughout the spatial domain. In these situations a combination of an intrusive and non-intrusive method can be beneficial and more efficient. In this work, we consider a coupling between an intrusive and non-intrusive method. The intrusive approach uses a combination of polynomial chaos and stochastic Galerkin projection. The non-intrusive method uses numerical integration by combining quadrature rules and probability density functions of the prescribed uncertainties. A provably stable coupling procedure between the two methods will be presented. The coupling procedure is constructed for a hyperbolic system of equations. The theoretical results are verified by numerical experiments.

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CP15

Utilizing Multisymmetry Properties in Uncertainty Quantification

Many interesting applications in physics that can be modeled by stochastic partial differential equations exhibit symmetries that can be exploited to reduce computational effort. The numerical solution of such problems requires the numerical integration of high-dimensional integrals, for example in stochastic collocation methods or Bayesian estimation.
Since the *curse of dimensionality* is encountered frequently in Uncertainty Quantification and problems turn out to be computationally highly demanding, we are interested in reducing the complexity of such problems. This can be achieved by making use of permutation-invariance properties in solution approaches, the most important example of such a property being multisymmetry.
Here we discuss extensions and applications of the ideas and techniques presented in our previous work on cubature formulas for multisymmetric functions, setting our focus on problems such as the solution of stochastic partial differential equations and introducing new ideas such as basis reduction techniques to adapt existing solution approaches to the idea of capitalizing on multisymmetry properties. We show with numerical examples that the presented approach is highly efficient compared to conventional methods that do not utilize multisymmetry properties.

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An Adaptive (Quasi-) Monte Carlo Method for Forward Uncertainty Quantification in Differential Equations with Random Coefficients

We present an adaptive (quasi-) Monte Carlo method for the solution of differential equations with random coefficients. The algorithm adaptively constructs an estimator for the expected value of some functional of the solution until an user-specified tolerance is satisfied. The performance of the algorithm is studied. The efficiency of Monte Carlo and quasi-Monte Carlo method is compared.

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CP16

Aeroacoustics of Cavity Flow Analyzed with Multilevel Monte Carlo and Non-intrusive Polynomial Chaos Methods

In this presentation, we apply two non-intrusive uncertainty propagation methods to aeroacoustic simulations with uncertain input, exemplified by noise generation in cavity flow. The noise generated via Rossiter modes and turbulent rumble is particularly relevant, for example in automobile exterior aerodynamics. The underlying deterministic large eddy simulations are carried out using a discontinuous Galerkin (DG) method solving the full compressible Navier-Stokes equations, where the aeroacoustic sources are directly resolved. We first apply the multilevel Monte Carlo (MLMC) method to this problem setting. The high spatial and temporal order of the employed DG discretization have several important implications for the MLMC framework: In turbulent flow, the theoretical convergence order of the DG method is not reached. An empirical update at runtime of the estimated stochastic level errors and optimal number of samples on each level become necessary. Level convergence is not always obtained, and depends on the chosen quantity of interest. In a high-order environment, different grid resolutions can be achieved through both h- and p-refinement. Here, we use a combined h-p-refinement. We validate the method by comparing convergence rates and efficiency to results obtained with a non-intrusive polynomial chaos method with a sparse grid approach. We also identify the most influential input parameters for cavity flow noise generation.

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CP16

Uncertainty Quantification of Rans Turbulence Models Using Bayesian Deep Learning with Stein Variational Gradient Descent

The Reynolds-averaged Navier-Stokes (RANS) is one of the most commonly used CFD methods due to its low computational cost and ability ?to handle extremely high Reynolds numbers. ?A parametrized turbulence model is introduced ??resulting in significant uncertainties ?in the simulation results. ? In recent years, machine learning approaches have become essential for considering model error and ? uncertainty quantification ?in RANS simulations? and to improve turbulence modeling. In this work, we ?present a? ?Bayesian ?deep learning? approach using ? ?Stein Variational gradient descent ? ?to quantify model uncertainties in RANS. We train our model using a set of simple flows with several different geometries with high-fidelity ?simulations??. We ?demonstrate the predictive capability of the model as well as its ability to accurately compute flow statistics using limited training data.

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CP16

Application of Machine Learning Algorithms for the Classification of Regions of RANS Discrepancy

Reynolds Averaged Navier Stokes models represent the workhorse for industrial research and design, with a vast majority of such turbulence simulations utilizing RANS models. Owing to the assumptions and simplifications utilized during their formulation, RANS models introduce a significant measure of model form uncertainty in the simulation results. To establish RANS models as reliable tools in engineering design, there is a need for accurate quantification of these discrepancies. Recent work using eigenspace perturbations has shown significant promise is providing such uncertainty bounds. However, at present, such methods have to cater to a worst case scenario and apply the maximally permissible perturbation, at all points in the flow. Bereft of a spatial marker function for RANS uncertainty, the eigenspace perturbation methods tend to overestimate the predictive discrepancy. We apply, appraise

and analyze the efficacy of select data driven algorithms to formulate universal marker functions. In this talk, we compare and contrast the results from Random Forests, Support Vector Machines and Adaboost decision trees. The training sets included a database of canonical flow configurations. Using these, classifiers were developed for each different nature of projection, assigning each point in the computational domain into a specific class. We exhibit that these classifiers are robust and are able to generalize to flows significantly different from the training set.

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CP16

Physics-Derived Approaches to Multi-physics Model Form Uncertainty Quantification: Application to Turbulent Combustion Modeling

The major challenge in multi-physics modeling is the sheer number of models, across multiple physical domains, that are invoked, each of which involves its own set of assumptions and subsequent model errors. Quantification of model errors, that is, model form uncertainty quantification, is critical in assessing which model dominates the total uncertainty and should be targeted for improvements. The fundamental challenge in quantifying model error is in translating model assumptions, inherently coupled to the physics, into mathematical statements of uncertainty. In this work, two methods are presented for deriving model error estimates directly from the physics, bypassing the need for training data. The first method, peer models, uses models with differing assumptions to derive an uncertainty estimate. This peer model approach relies on model variability as an estimate for model error, which is determined from what can be reasonably assumed about the underlying physics to be modeled. The second method, hierarchical models, uses a higher-fidelity model to estimate the uncertainty in a lower-fidelity model. This hierarchical approach can be leveraged as the basis for an uncertainty-adaptive modeling approach that minimizes computational effort given an acceptable model error threshold. These approaches to model form uncertainty quantification are applied within the context of Large Eddy Simulation (LES) modeling of turbulent combustion.

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CP16

Uncertainty Quantification of Rans Initialization in Modeling Shock-driven Turbulent Mixing

As we know the initial conditions play a role in modeling of RANS. In this talking we quantify initial-data uncertainties in simulation of the inverse chersov shock tube. A high order finite volume multi-component flow simulating model is coupled with a polynomial chaos to propagate the initial-data uncertainties to the system quantities of interest. The results shows that the initial condition is highly influencing to the mixing process.

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CP17

On the Accuracy of Free Energy Defect Computations in Atomistic Systems

The macroscopic behavior of a crystalline material is strongly dependent on the type and distribution of defects present. This talk describes the analysis of the free energy of defect formation for the model problem of a constrained 1D system, and its convergence properties in the thermodynamic limit.

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CP17

Addressing Global Sensitivity in Chemical Kinetic Models using Adaptive Sparse Grids

Chemical kinetic models often carry very large parameter uncertainties and show a strongly non-linear response with rapid changes over relatively small parameter ranges. In addition, the dimensionality of the parameter space can grow to a large number, without a priori known structure between the dimensions. Using a real life model for the water splitting on a Cobalt oxide catalyst as a prototypical example, we demonstrate an adaptive sparse grid strategy (ASG) for the global sensitivity analysis of such models based on the Analysis Of Variances. The ASG utilizes local adaptivity, to address the rapid changes, as well as dimension adaptivity, to exploit the typical intrinsic low dimensional parameter dependence in reaction networks. We will discuss, how ASG can be extended to a multilevel strategy, when the model response is not deterministic but must be obtained from sampling a stochastic model.

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CP17

Providing Structure to Experimental Data: A Large-Scale Heterogeneous Database for Collaborative Model Validation

Experimental data is often stored in various file formats and unfortunately, requires highly specialized codes to parse each individual set of data. The lack of a structured format makes it challenging to find relevant experimental data across a diverse collection for model validation and uncertainty quantification (V/UQ). The PrIMe Data Warehouse (http://primekinetics.org) has open and flexible data models which provide much-needed structure to experimental data by using standard XML files. Every data value is distinctly labeled, making it simple to search for and make use of data from several sources

through a single search query. Recent additions of thousands of coal devolatilization and oxidation experiments highlighted the flexibility of the PrIMe data models, enabling researchers to quickly incorporate validation data from different sources in their V/UQ analysis. We will present an example utilizing the experimental data from PrIMe to validate a reduced char oxidation physics model. A Bound-to-Bound Data Collaboration consistency analysis will be used for validation of the char oxidation model with data in both air and oxy-coal conditions. Uncertainty in the kinetic rate parameters between char carbon and O_2, H_2O, and CO_2 will also be quantified.

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CP17

On the Fly Coarse-graining in Molecular Dynamics Simulations

We present a general framework for enhancing sampling of highly complex distributions e.g. occurring in peptide simulations having several local free-energy minima by biasing the dynamics and learning a probabilistic coarse-grained (CG) model simultaneously. Its main component represents a bayesian CG model which is learned on the fly during the simulation of the target distribution. We in turn use insights, gathered from that CG model, to bias the fine-grained potential in order to enhance the exploration of the configurational space and overcome high energy barriers. Next to biasing dynamics, the CG model serves as probabilistic predictor while we quantify the predictive uncertainty arising due to information loss from coarse-graining. An important component of the presented methodology builds the coarse-to-fine mapping which implicitly extracts, without any physical insight, lower dimensional collective variables, the CG variables. We propose a mixture model serving as coarse-to-fine mapping while we sequentially add mixture components and increase the mappings flexibility. Moreover, the complexity of the employed components is consecutively increased by adding features based on an information theoretic metric. We demonstrate the capabilities of the proposed methodology in the context of peptide simulations.

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CP18

Bayesian Calibration for Models with Nonlinear Inequality Parameter Constraints

This work is focused on developing a Bayesian calibration technique to probabilistically characterize models whose parameters are governed by nonlinear inequality constraints. While Bayesian model calibration has become increasingly popular, the state-of-the-art methods experience limitations for models with constrained parameters. The proposed technique builds the joint posterior distribution of the parameters entirely within the feasible parameter space defined by the given constraints. This is accomplished through an enrichment of the Hamiltonian Monte Carlo (HMC) sampling technique, part of the Markov Chain Monte Carlo family of methods, in which any arbitrary parameter constraints (e.g., linear or nonlinear inequalities) are evaluated during sampling. In HMC, the system of equations describing Hamiltonian dynamics simulate the evolution of a Markov chain; the constraint evaluation is directly embedded into the solution of that system of equations. Thus, the proposed method offers an intrinsic enforcement of constraints, in contrast to traditional means of extrinsic enforcement. The proposed technique is demonstrated through an application to a constitutive model for hyperelasticity that is calibrated using experimental data of brain tissue from two distinct studies. The constitutive model parameters are constrained by the Drucker stability criterion, which restricts the softening behavior of hyperelastic models to ensure the physical meaningfulness of their predictions.

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CP18

Inverse Uncertainty Quantification Applied to an Industrial Model with Measurement Data

The demand on reliable information about complex physical and computational simulation models is continuously increasing. In an industrial context the use of uncertainty quantification (UQ) methods gain more and more relevance and one integral part consists of evaluating distributions on parameters for those models. The contribution presents an electric drive with a test bench hardware which allows to generate systematic measurements with underlying uncertainties. The distributions of the parameter uncertainties are in general unknown in advance but can be defined by means of adequate tuning of the test bench. This knowledge can be used afterwards to validate the approach. In this context, Bayesian inference is applied to estimate the parameter distributions based on a detailed simulation model and the recorded measurement data. The results are obtained by a Markov Chain Monte Carlo (MCMC) method in combination with a Polynomial Chaos (PC) surrogate model. Our focus is to extract relevant parts of the measurement data to compose a likelihood function, which contains the required information. Labelling the measurement parts is done using a global sensitivity analysis based on Sobol' indices gained from the PC coefficients. The approximated parameter uncertainties are compared to the real values of the test bench hardware and an outlook of scalability and applicability for industrial models with fo-

cus on mechatronic systems is provided.

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CP18

Simulation-based Uncertainty Quantification for Atmospheric Remote Sensing Retrievals

Earth-observing satellites provide substantial volumes of data with comprehensive spatial and temporal coverage that inform many environmental processes. The operational processing of remote sensing data often must be computationally efficient to make data products available to the scientific community in a timely fashion. This is particularly true for an inverse problem that is known as a remote sensing retrieval, which is the process of producing estimates of geophysical quantities of interest from satellite observations of reflected sunlight. There are several classes of retrieval algorithms, and this work highlights a common probabilistic framework for quantifying uncertainty imparted by choices made in the retrieval process. We illustrate tools for investigating retrieval error distributions from Monte Carlo experiments applied to retrievals of atmospheric temperature, water vapor, and trace gas concentrations.

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CP18

Bayesian Calibration of Expensive Computer Models with Input Dependent Parameters

Computer models, aiming at simulating complex physical procedures, often involve complex parametrisations whose optimal parameter values may be different at different model input values. Traditional model calibration methods cannot address such cases because they assume that these optimal values are invariant to the inputs. We present a fully Bayesian methodology which is able to produce input dependent optimal values for the calibration parameters, as well as it characterizes the associated uncertainties via posterior distributions. A particular highlight of the method is that it can also address problems where the computer model requires the selection of the sub-model from a set of competing ones, but the choice of the best sub-model may change with respect to the input values. Central to the methodology is the idea of modelling the unknown model parameter as binary treed process whose index is the model input, and specifying a hierarchical prior model. Suitable reversible jump operations are proposed to facilitate the challenging computations. The performance of the method is assessed against a benchmark example. We apply our method to to address a real application, with a large-scale climate model, where interest lies on the selection of different sub-models at different spatial regions.

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CP18

Spatial Statistical Downscaling for Constructing High-resolution Nature Runs in Global Observing System Simulation Experiments

Observing system simulation experiments (OSSEs) have been widely used as a rigorous and cost-effective way to guide development of new observing systems, and to evaluate the performance of new data assimilation algorithms. Nature runs (NRs), which are outputs from deterministic models, play an essential role in building OSSE systems for global atmospheric processes because they are used both to create synthetic observations at high spatial resolution, and to represent the "true' atmosphere against which the forecasts are verified. However, most NRs are generated at resolutions coarser than actual observations. Here, we propose a principled statistical downscaling framework to construct high-resolution NRs via conditional simulation from coarse-resolution numerical model output. We use nonstationary spatial covariance function models that have basis function representations. This approach not only explicitly addresses the change-of-support problem, but also allows fast computation with large volumes of numerical model output. We also propose a data-driven algorithm to select the required basis functions adaptively, in order to increase the flexibility of our nonstationary covariance function models. In this article we demonstrate these techniques by downscaling a coarse-resolution physical NR at a native resolution of 1° latitude $\times$ 1.25° longitude of global surface CO_2 concentrations to 655,362 equal-area hexagons.

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CP18

Mean-based Preconditioning for the Helmholtz Equation in Random Media

The Helmholtz equation models single-frequency acoustic

waves and is challenging to solve numerically even in the abscence of randomness. As a result, the matrices arising from finite element discretisations of the Helmholtz equation, especially for high-frequency waves, require preconditioning. However, when solving a forward UQ problem using a Monte Carlo-type method, using a different preconditioner for each realisation of the random medium is infeasible. In our mean-based preconditioning strategy, we calculate a preconditioner based on the mean of the random medium, and then use this preconditioner for all the linear systems arising from the realisations of the random medium. We present a general class of random media for which we can prove an a priori bound on the solution of the Helmholtz equation. For these media we can prove that our mean-based preconditioning strategy is accurate, and we present computations confirming this. We also present computations indicating that our method is accurate for a wider class of random media than those supported by theoretical results. This preconditioning strategy also gives rise to a technique for increasing the speed of MCMC procedures for the statistical inverse problem, which is of interest in imaging and geophysics. We also discuss new results about the equivalence of the different possible formulations of the forward problem, with these underlying the theoretical results above.

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CP19

Design of Experiments-based Geological Uncertainty Quantification of Co2-Assisted Gravity Drainage (gagd) Process in Heterogeneous Multilayer Reservoirs

The Gas-Assisted Gravity Drainage (GAGD) process results in better sweep efficiency and higher microscopic displacement to enhance the bypassed oil recovery. Unlike the conventional gas injection, the GAGD process takes advantage of natural reservoir fluids segregation to provide gravity stable oil displacement. It consists of placing a horizontal producer near the bottom of the pay zone and injecting gas through vertical wells. The GAGD process was evaluated considering high-resolution compositional reservoir model that includes 3D lithofacies and petrophysical property distribution. Three quantiles of P10, P50, and P90 were incorporated in reservoir model along with Design of Experiments (DoE) to study the heterogeneity and anisotropy effects on the GAGD process. The parameters are horizontal permeability, anisotropy ratio, pore compressibility, effective reservoir porosity, aquifer size, in addition to CO2 injection rate, maximum oil production rate, minimum BHP in horizontal producers, and maximum BHP in injection wells. Experimental Design has led to determine the most dominant factors affecting the GAGD performance. Among all the different property realizations, it was clearly seen that anisotropy ratio has direct impact on the process as the 3D lithofacies modeling included Sand, Shaly Sand, and Shale that impede the vertical fluids movement; however, the immiscible CO2 injection indicated the insensitivity of the GAGD process to reservoir heterogeneities.

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CP19

Uncertainty Quantification of Textile Composites: A Multi-Scale Approach

Stochastic analysis has been performed in a multi-scale framework to study the resulting deformation characteristics and bending stresses of laminated woven composites. To this end, a novel adaptive sparse locally refined metamodel based uncertainty quantification (UQ) framework has been developed for response approximation, considering stochastic micro-mechanical and geometric properties. Sensitivity analysis has been carried out to ascertain the influence of stochastic parameters on the output. In context to the undertaken multi-scale structural application, a 3-D elasto-plastic constitutive model of graphite-epoxy plain woven composite has been developed. Analysis has been performed using both asymptotic and analytical mean field homogenization techniques. As a practical real-life application, a macro-scale finite element model of laminated woven composite has been developed and analyzed using properties obtained from micro-scale to predict response characteristics of a wind turbine rotor blade subjected to various realistic in-plane and out-of-plane loading. The significance of the study lies in the fact that stochasticity in micro-structural attributes have strong influence on the system performance. Therefore, to ensure robustness and reliability of large-scale structures, it is crucial to account such forms of uncertainties and realistic multi-scale modelling techniques.

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CP19

Sensitivity Analysis and Data Assimilation for Fracture Simulations Model

Fracture propagation plays a key role for a number of applications of interest to the geophysical community. In this work we implement a global sensitivity analysis test as well as data assimilation to the Hybrid Optimization Software Suite (HOSS), a multi-physics software tool based on the combined finite-discrete element method, that is used to describe material deformation and failure. We implement the Fourier Amplitude Sensitivity Test (FAST) to explore how each parameter influence the model fracture and to determine the key model parameters that have the most impact on the model. Based on the results from the sensitivity analysis we implement a Gaussian Mixture Model (GMM) assimilation method to determine the best parameter values to match different experimental data. The GMM are assimilation methods that are able to effectively represent the probability density function of non-linear models through a mixture of Gaussian functions. The results show a good agreement between assimilated model simula-

tion and experimental data from Split Hopkinson Pressure Bar (SHPB) experiments.

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CP19

Derivative-based Expression of Sobol's Total Index

A deep exploration of mathematical complex models is often made by using model-free methods. Variance-based sensitivity analysis, Derivative-based sensitivity analysis, and multivariate sensitivity analysis (MSA) are ones of them. In one hand, variance-based sensitivity analysis (VbSA) allows for assessing the effects of inputs on the model outputs, including the order and the strength of interactions among inputs. On the other hand, Derivative-based sensitivity measure (DGSM), which is computationally more attractive than VbSA, provides only the global effect of inputs. It is worth interesting to combine the advantages of both methods and to come up with a new approach. So far, the upper and lower bounds of Sobol' indices have been investigated. The upper bound of the Sobol total index is a (known) constant times the DGSM index. Thus, a small value of the upper bound of the Sobol total index means that the associated input does not act in the model. However, a big value does not bring much information, regarding factors classification. In this abstract, we provide a new mathematical expression of Sobol's total index based on model derivatives for any probability distribution of inputs that is dominated by the Lebesgue measure. The new expression of the Sobol total index is a function of model partial derivatives, the density function, and the the cumulative distribution function of a given input.

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CP20

Uniform Sampling of a Feasible Set of Model Parameters

Physically based modeling of complex systems usually leads to a large dimensionality in the parameter space. Uncertainties are in general inevitable for those parameters. Quantification of uncertainty is therefore crucial for developing predictive models. Bound-to-Bound Data Collaboration (B2BDC) is a systematic methodology that combined model and data to evaluate and ultimately reduce the joint uncertainty of model parameters. The feasible set is defined as the region in the parameter space that is consistent with the experimental data. The ability of generating uniformly distributed samples within the feasible set allows stochastic representation of the region of interest. Despite the successful development and elegant format of different sampling methods, their performance in large-scale realistic situations becomes computationally limited. Here, we present an acceptance-rejection sampling approach aided by approximation strategy and dimension reduction. The method offers uniformly distributed samples in low-dimensional applications and good approximations in high-dimensional cases, with a tractable computational expense. Quantitative analysis demonstrates efficiency-accuracy trade-off of the approach. The method is also compared to the Adaptive Metropolis (AM) sampling method and showed better computational performance in several test cases.

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CP20

Distribution Surrogates for Efficient UQ in Multi-physics Problems

Multi-physics analysis under uncertainty can be computationally expensive since it involves a nested double-loop analysis, where the multidisciplinary analysis is carried out in the innermost loop, and uncertainty analysis in the outer loop. In some applications (e.g., automotive or aerospace vehicle design), there is also a third optimization loop. To alleviate the high computational expense, this talk presents a novel distribution surrogate-based approach, which helps collapse the traditional nested simulation process by enforcing the multi-physics compatibility condition simultaneously within the uncertainty analysis. A distribution surrogate directly provides the probability distribution of the output as opposed to a deterministic surrogate, which provides a point value of the output at any given input and requires multiple runs. Multi-physics analysis under uncertainty involves both forward prediction and inference since system output computation at any input requires the satisfaction of multidisciplinary compatibility. Several distribution surrogates, with and without analytical inference, such as multivariate Gaussian, Gaussian copula, Gaussian mixture and Bayesian network are discussed, and their performance, in terms of modeling effort and prediction accuracy, are compared against Monte Carlo results of fully coupled multi-physics simulations.

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CP20

Looking the Wrong Way: Beyond Principal Components in Computer Model Calibration

When faced with large spatio-temporal computer model output, calibration is commonly performed by projecting the data onto a principal component (PC) basis derived from the ensemble, before emulators are constructed for the coefficients on this basis (Higdon et al 2008). This has become the standard approach in UQ for high-dimensional output (e.g. climate models). However, this is flawed when the ensemble, and hence the PC basis, does not contain the key patterns from the observed data we are attempting to calibrate the model to. We show that in this case, we guarantee the conclusion that the computer model cannot accurately represent the observations up to model discrepancy

(what we term the 'terminal case'), regardless of whether this is true. This problem has been evident in every climate field we have encountered, highlighting the prevalence and importance of this problem. We present a methodology for optimal projection-based computer model calibration for high-dimensional model output that overcomes this flaw in existing approaches. Our method consists of a simple test allowing us to identify whether we are in the terminal case, and provides an efficient algorithm for overcoming this problem via an optimal rotation of the PC basis. This allows important directions or patterns in the output space (i.e. those more similar to the observations) to be incorporated into the basis, enabling input parameters leading to the observations to be identified, should they exist.

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CP20

Fourier Decomposition Methods for Efficient Generation of Random Fields

Fourier methods for the representation of random fields and sample generation enjoy widespread use for their simplicity and efficient implementation when FFT methods are employed (e.g. in the form of circulant embeddings). However, their use is mostly restricted to rectangular domains and sampling-based methods (e.g. MC, QMC). For spectral methods on non-rectangular domains only little has been done so far. In this talk, we want to take a deeper look into the application of Fourier methods for spectral stochastic methods on arbitrary domains. Furthermore, it will be shown how to use the Fourier decomposition of the covariance kernel in order to accelerate the computation of the Karhunen-Love expansion (KLE).

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CP20

On the Quantification and Propagation of Imprecise Probabilities in High Dimensions with Dependencies

As a generalized probability theory, imprecise probability allows for partial probability specifications and is applicable when data is so limited that a unique probability distribution cannot be identified. The primary research challenges in imprecise probabilities relate to quantification of epistemic uncertainty and improving the efficiency of uncertainty propagation with imprecise probabilities particularly for complex systems in high dimensions, at the same time considering dependence among random variables. The classical approach to address variable dependence from limited information is to assume that the random variables are coupled by a Gaussian dependence structure and rely on a transformation into independent variables. This assumption is often subjective, inaccurate, and not justified by the data. Recently, a new UQ methodology has been developed by the authors for quantifying and efficiently propagating imprecise probabilities with independent uncertainties created by a lack of statistical data. In this work, we generalize this new UQ methodology to overcome the limitations of the independence assumption by modeling the dependence structure of high dimensional random variables using imprecise vine copulas. The generalized approach achieves particularly precise estimates for UQ and efficient uncertainty propagation of imprecise probabilities in high dimensions with dependencies.

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MS1

Episodic, Non-linear and Non-Gaussian: Uncertainty Quantification for Cloud, Precipitation, Fire and Ice

The uncertainty distributions of forecasts of episodic variables such as clouds, precipitation, fire and ice often feature a finite probability of non-existence and/or skewness. Furthermore, many of these variables feature strongly nonlinear dynamics. For such variables, existing data assimilation techniques such as 4DVAR, the Ensemble Kalman Filter (EnKF) and the Particle Filter (PF) fail when a finite amount of the variable is observed but the prior forecast uncertainty distribution assigns a probability density of zero to this observation. Here we extend the previously developed Gamma, Inverse-Gamma and Gaussian (GIGG) variation on the EnKF to accommodate finite probabilities of non-existence. The resulting GIGG-Delta filter has the remarkable property that when rain (for example) is observed, the GIGG-Delta filter always produces a posterior ensemble of raining ensemble members even if not one of the prior forecast ensemble members contain rain. In addition, the GIGG-Delta filter accurately solves Bayes theorem when the prior and observational uncertainties are given by gamma and inverse-gamma pdfs, respectively. To account for non-linearity, a new iterative balancing procedure is proposed that improves the ability of the EnKF to produce balanced posterior states. The approach is tested, illustrated and compared with existing techniques using a hierarchy of idealized models.

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MS1

Reducing Precision in Ensemble Data Assimilation to Improve Forecast Skill

We present a new approach for improving the efficiency of data assimilation, by trading numerical precision for computational speed. Future supercomputers will allow a greater choice of precision, so that models can use a level of precision that is commensurate with the model uncertainty. Data assimilation is inherently uncertain due to the use of relatively long assimilation windows, noisy observations and imperfect models. Thus, the larger rounding errors incurred from reducing precision may be within the tolerance of the system. Lower precision arithmetic is cheaper, and so by reducing precision in ensemble data assimilation, we can redistribute computational resources towards, for example, a larger ensemble size. We will present results on how lowering numerical precision affects the performance of an ensemble data assimilation system, consisting of the SPEEDY intermediate complexity atmospheric model and the local ensemble transform Kalman filter. We will reduce the precision of the system beyond single precision

(using an emulation tool), and compare the results with simulations at double precision. The lowest level of precision is related to the level of uncertainty present: with greater uncertainty, precision is less important. Additionally, by reinvesting computational resources from lowering precision into the ensemble size, higher skill analyses and forecasts can be achieved.

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MS1

Balanced Data Assimilation for Highly-Oscillatory Mechanical Systems

We apply data assimilation algorithms to highly-oscillatory Hamiltonian systems with state variables that act on different time scales. There exist certain balance relations between those variables and if they are nonlinear, the linear structure of LETFs (linear ensemble transform filters) results in violations of those relations and therefore spurious oscillations on the fast time scale are excited. We present two strategies to deal with that issue. One addresses the problem by blending between different models during the time-stepping in the forecast part of the sequential data assimilation algorithm. The other one minimises a cost functional including the residual of the balance relation as a penalty term after the performance of the filtering step. We test both methods on two different scenarios: a highly oscillatory Hamiltonian system and a thermally embedded highly oscillatory Hamiltonian system. The results of the experiments show that we are able to drastically reduce the spurious oscillations in all cases.

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MS1

Singular Likelihoods to Prevent Particle Filter Collapse

Particle filters are a method for nonlinear, non-Gaussian data assimilation and uncertainty quantification. They operate by assigning positive weights to members of an ensemble of forecasts based on how close the ensemble members are to observations. Unfortunately particle filters typically require an impossibly high number of ensemble members to avoid 'collapse': a single member having essentially all the weight, and the others having none. This talk presents a method to reduce the ensemble size required for particle filters. It measures the 'distance' of an ensemble member to the observations using a metric that de-weights errors at small scales. This is tantamount to describing the observation error as a generalized random field. Huge performance improvements compared to standard implementations are shown in a simple example.

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MS2

Mutual Information-based Experimental Design for Problems in Nuclear Engineering

In this presentation, we will discuss the use of a mutual information-based experimental design framework to employ validated high-fidelity codes to calibrate low-fidelity codes and guide moving sensor strategies. For the first problem, one objective is to specify where in the design space high-fidelity codes should be evaluated to maximize information pertaining to low-fidelity model parameters. A theoretical issue, which we will discuss, entails the development of algorithms that accommodate the inherent correlation between parameters and responses. We will demonstrate the performance of these algorithms for thermal-hydraulics and fuels codes employed when simulating light water reactor designs. We will additionally discussion how the mutual information-based framework can be employed to guide moving sensors to determine the location and intensity of radiation sources in an urban environment.

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MS2

Mutual Information Estimation in High Dimensions

Mutual information is the most common maximization criteria in optimal experimental design as it is a natural measure of dependence between two random variables. However, the estimation of mutual information in high dimensions remains a challenge. Initial results are presented in replacing the estimation of mutual information in high dimensions with a distance measure in low dimensions.

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MS2

Optimal Experimental Design for Prediction Using a Consistent Bayesian Approach

Experimental data is often used to infer valuable information about parameters for models of physical systems. However, the collection of experimental data can be costly and time consuming. In such situations we can only afford to gather some limited number of experimental data, however not all experiments provide the same amount of information about the processes they are helping inform. Consequently, it is important to design experiments in an optimal way, i.e., to choose some limited number of experimental data to maximize the value of each experiment. Moreover, the optimality of the experiment must be chosen with respect to the penultimate objective. We present an efficient approach for optimal experimental design based on a recently developed consistent Bayesian formulation. We demonstrate that the optimal design depends on whether we are primarily interested in inference of parameters or the prediction of quantities of interest that cannot be observed directly. Numerical results will be presented to illustrate both types of optimal experimental design and to highlight the differences.

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MS2

Solving Integer Programming Problems in Design of Experiments

We present a numerical method for approximating the solution of convex integer programs stemming from optimal experimental design. The statistical setup consists of a Bayesian framework for linear inverse problems for which the direct relationship is described by a discretized integral equation. Specifically, we aim to find the optimal sensor placement from a set of candidate locations where data are collected with measurement error. The convex objective function is a measure of the uncertainty, described here by the posterior covariance matrix, of the discretized linear inverse problem solution. The resulting convex integer program is relaxed producing a lower bound. An upper bound is obtained by extending the sum-up rounding approach to multiple dimensions. For this extension, we provide an analysis of its accuracy as a function of the discretization mesh size. We show asymptotic optimality of the integer solution defining the upper bound for different experimental design criteria (A, D, E - optimal), by proving the convergence to zero of the gap between upper and lower bounds as the mesh size goes to zero and the number of candidate locations goes to infinity in a fixed proportion to the total number of mesh points. The technique is demonstrated on a two-dimensional gravity surveying problem for both A-optimal and D-optimal sensor placement where our designs yield better procedures compared to random placements.

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MS3

Randomized Newton and Quasi-Newton Methods for Large Linear Least Squares Problems

We discuss randomized Newton and randomized quasi-Newton approaches to efficiently solve large linear least-squares problems where the very large data sets present a significant computational burden (e.g., the size may exceed computer memory or data are collected in real-time). In our proposed framework, stochasticity is introduced in two different frameworks as a means to overcome these computational limitations, and probability distributions that can exploit structure and/or sparsity are considered. Our results show, in particular, that randomized Newton iterates, in contrast to randomized quasi-Newton iterates, may not converge to the desired least-squares solution. Numerical examples, including an example from extreme learning machines, demonstrate the potential applications of these methods.

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MS3

A Probabilistic Subspace Bound, with Application to Active Subspaces

We analyze a dimension reduction approach for the identification of response surfaces. Given a function f that depends on m parameters, one wants to identify a low-dimensional "active subspace" along which f is most sensitive to change, and then approximate f by a response surface over this active subspace. More specifically, let $X \in \mathbb{R}^m$ be random vectors corresponding to a probability density $\rho(x)$, and let E be the expected value of the "squared" gradient of $f(X)$. An "active subspace" is an eigenspace associated with the strongly dominant eigenvalues E. To reduce the cost, we compute the eigenspace instead from a Monte Carlo approximation S. We present bounds on the number of Monte Carlo samples so that, with high probability, the angle between the eigenspaces

of E and S is less than a user-specified tolerance. Our probabilistic approach resembles the low-rank approximation of kernel matrices from random features, but with more stringent accuracy measures. Our bounds represent a substantial improvement over existing work: They are non-asymptotic; fully explicit; allow tuning of the success probability; and do not depend on the number m of parameters, but only on the numerical rank (intrinsic dimension) of E. They also suggest that Monte Carlo sampling can be efficient in the presence of many parameters, as long as the underlying function f is sufficiently smooth.

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MS3

Recovery from Random Observations of Non-linear Low-rank Structures

Abstract not available at time of publication.

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MS3

Maximize the Expected Information Gain in Bayesian Experimental Design Problems: A Fast Optimization Algorithm Based on Laplace Approximation and Randomized Eigensolvers

Optimal experimental design (OED) for Bayesian nonlinear inverse problems governed by partial differential equations (PDEs) is an extremely challenging problem. First, the parameter to be inferred is often a spatially correlated field and it leads after discretization to a high dimensional parameter space. Second, the forward model is often extremely complex and computationally expensive to solve. A common objective function for OED is the expected information gain (EIG). Naïve evaluation of EIG is unfeasible for large-scale problems due to the large number of samples required in the double-loop Monte Carlo. To overcome these difficulties, we invoke an approximation of the EIG based on the Laplace approximation of the posterior. Each evaluation of the objective function then requires computing a sample average approximation (over possible realization of the data) of the information gain (IG) between the Laplace approximation and the Gaussian prior distribution. An analytical formula for the IG is available and it involves the log-determinant and trace of the posterior covariance operator. Randomized eigensolver algorithms allows us to efficiently estimate such invariants at a cost that is independent of the dimension of the parameter space, thus allowing for a scalable evaluation of the objective function. Variational adjoint methods are then used to efficiently compute the gradient of the OED objective function. An application to inverse scattering will be presented.

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MS4

Approximate Integral Methods for Fast Model Diagnostics

Nuisance parameters increase in number with more observations making them impossible to scale to realistic problems. One way to make estimation possible for these models is to marginalize out nuisance parameters thereby reducing the effective dimension of the model. Since accurate high dimensional numerical integration is unfeasible, the standard tool for marginalization is to apply the Laplace Approximation, a second order Taylor expansion enabling the required high dimensional integral to be approximated as the kernel of a Gaussian density. While this makes the estimation of structural parameters feasible it comes with a heavy assumption which is asymptotically correct. The problem is that the required asymptotics are unattainable on the nuisance parameters for which the approximation is applied. In this talk we present a probabilistic integration tool as a fast diagnostic assessment of the validity of the Laplace approximation. Furthermore, we showcase how to fold the probabilistic integrator into the marginalization and estimation methodology.

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MS4

Bayesian Probabilistic Numerical Methods for Industrial Process Monitoring

The use of high-power industrial equipment, such as large-scale mixing equipment or a hydrocyclone for separation of particles in liquid suspension, demands careful monitoring to ensure correct operation. The task of monitoring the liquid suspension can be posed as a time-evolving inverse problem and solved with Bayesian statistical methods. In this paper, we extend Bayesian methods to incorporate statistical models for the error that is incurred in the numerical solution of the physical governing equations. This enables full uncertainty quantification within a principled computation-precision trade-off, in contrast to the over-confident inferences that are obtained when numerical error is ignored. The method is cast with a sequential Monte Carlo framework and an optimised implementation is provided in Python.

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MS4

Convergence Rates of Gaussian ODE Filters

A recently introduced class of probabilistic (uncertainty-aware) solvers for ordinary differential equations (ODEs) employs Gaussian (Kalman) filtering to solve initial value

problems. These methods model the true solution x and its first q derivatives *a priori* as a Gauss–Markov process X, which is then iteratively conditioned on information on $\dot{x}$ from evaluations of f. We prove local convergence rates of order h^{q+1} for all previously introduced versions of this Gaussian ODE filter, as well as global convergence rates of order h^1 in the case of $q = 1$, integrated Brownian motion prior and maximum a posteriori measurement model, and provide precision/uncertainty requirements on evaluations of f for these rates. Thereby, this paper removes multiple restrictive assumptions for these local convergence rates, and provides a first global convergence result for Gaussian ODE filters as well as a first analysis for the explicit incorporation of evaluation uncertainty in such models.

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MS4

Bayesian Probabilistic Numerical Methods

Numerical computation — such as numerical solution of a PDE — can modelled as a statistical inverse problem in its own right. The popular Bayesian approach to inversion is considered, wherein a posterior distribution is induced over the object of interest by conditioning a prior distribution on the same finite information that would be used in a classical numerical method, thereby restricting attention to a meaningful subclass of probabilistic numerical methods distinct from classical average-case analysis and information-based complexity. The main technical consideration here is that the data are non-random and thus the standard Bayes' theorem does not hold. General conditions will be presented under which numerical methods based upon such Bayesian probabilistic foundations are well-posed, and a sequential Monte-Carlo method will be shown to provide consistent estimation of the posterior. The paradigm is extended to computational "pipelines', through which a distributional quantification of numerical error can be propagated. A sufficient condition is presented for when such propagation can be endowed with a globally coherent Bayesian interpretation, based on a novel class of probabilistic graphical models designed to represent a computational work-flow. The concepts are illustrated through explicit numerical experiments involving both linear and non-linear PDE models.

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MS5

Speeding Up Sequential Tempered MCMC for Fast Bayesian Inference and Uncertainty Quantification

Bayesian methods are critical for quantifying the behaviors of complex physical systems. In this approach, we capture our uncertainty about a system's properties using a probability distribution and update this understanding as new information becomes available. We can then also make probabilistic predictions that incorporate uncertainties to evaluate system performance and make decisions. While Bayesian methods are critical, they are often computationally intensive, particularly for posterior uncertainty quantification, which necessitates the development of new approaches and algorithms. In this talk, I will discuss my contributions to a family of population MCMC algorithms, which I call Sequential Tempered MCMC (ST-MCMC) algorithms. These algorithms combine 1) a notion of tempering, to gradually transform a population of samples from the prior to the posterior through a series of intermediate distributions, 2) importance resampling, and 3) MCMC for the parallel sample chains. Using the sample population and prior information, we can adapt the proposal distribution to better utilize global information about the posterior as the ST-MCMC algorithm evolves. This enables faster sampling compared to standard implementations of ST-MCMC like methods. I will then illustrate the application of theses algorithms to problems in Bayesian inference, model selection, and posterior reliability assessment.

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MS5

Implicit Sampling for Stochastic Differential Equations

Monte Carlo algorithms that generate weighted samples from a given probability distribution, often known as importance samplers, are used in applications ranging from data assimilation to computational statistical mechanics. One challenge in designing weighted samplers is to ensure the variance of the weights, and that of the resulting estimator, are well-behaved. Recently, Chorin, Tu, Morzfeld, and coworkers have introduced a novel class of weighted samplers called implicit samplers, which possess a number of nice properties. This talk concerns an asymptotic analysis of implicit samplers in the small-noise limit. I will describe a simple higher-order implicit sampling scheme suggested by the analysis, and explain how it can be extended to stochastic differential equatons.

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MS5

Local Ensemble Kalman Filter with a Small Sample Size

Ensemble Kalman filter (EnKF) is an important data assimilation method for high-dimensional geophysical systems. Efficient implementation of EnKF in practice often involves the localization technique, which updates each component using only information within a local radius. We rigorously analyze the local EnKF (LEnKF) for linear systems, and show that the filter error can be dominated by the ensemble covariance, as long as 1) the sample size exceeds the logarithmic of state dimension and a constant that depends only on the local radius; 2) the forecast covariance matrix admits a stable localized structure. In particular, this indicates that with small system and observation noises, the filter error will be accurate in long time even if the initialization is not.

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MS6

A Variational Approach to Probing Extreme Events in Turbulent Dynamical Systems

Extreme events are ubiquitous in a wide range of dynamical systems, including turbulent fluid flows, nonlinear waves, large-scale networks, and biological systems. We propose a variational framework for probing conditions that trigger intermittent extreme events in high-dimensional nonlinear dynamical systems. We seek the triggers as the probabilistically feasible solutions of an appropriately constrained optimization problem, where the function to be maximized is a system observable exhibiting intermittent extreme bursts. The con- straints are imposed to ensure the physical admissibility of the optimal solutions, that is, significant probability for their occurrence under the natural flow of the dynamical system. We apply the method to a body-forced in- compressible Navier-Stokes equation, known as the Kolmogorov flow. We find that the intermittent bursts of the energy dissipation are independent of the external forcing and are instead caused by the spontaneous transfer of energy from large scales to the mean flow via nonlinear triad interactions. The global maximizer of the cor- responding variational problem identifies the responsible triad, hence providing a precursor for the occurrence of extreme dissipation events. Specifically, monitoring the energy transfers within this triad allows us to develop a data-driven short-term predictor for the intermittent bursts of energy dissipation. We assess the performance of this predictor through direct numerical simulations.

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MS6

Predictability of Extreme-causing Weather Patterns in the Midlatitude Turbulence

Blocking events are rare, large-scale, high-pressure (anticyclonic) weather systems that persist for more than five days and cause extreme events such as heat waves, cold spells, and extreme precipitation events. The underlying dynamics and the intrinsic predictability of blocking events are poorly understood and weather models have low prediction skills (compared to zonal flows) for these events. Recent studies have shown that blocking events arise from the internal dynamics of the tropospheric midlatitude turbulence and that ocean, topography, and other components of the Earth system play a secondary role. Building on these findings and recent progress in data-driven reduced-order modeling, we aim at studying predictability and prediction of blocking events. We employ a hierarchy of climate models, starting with a two-layer quasi-geostrophic (QG) model (the minimal physical model for these events) and an idealized global climate model (GCM). We conduct a perfect-model analysis in the QG model to determine the intrinsic predictability of blocking events and compare it with the predictability of zonal flows. We then apply a number of data-driven methods, based on Koopman operator and Fluctuation-Dissipation Theorem, and to the QG and GCM simulations seek to identify local or global patterns that provide short-term prediction skills for blocking events.

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MS6

New Statistically Accurate Algorithms for Fokker-Planck Equations in Large Dimensions and Predicting Extreme Events

Solving the Fokker-Planck equation for high-dimensional complex dynamical systems is an important issue. In this talk, efficient statistically accurate algorithms are developed for solving both the transient and the equilibrium solutions of Fokker-Planck equations associated with high-dimensional nonlinear turbulent dynamical systems with conditional Gaussian structures, which contain many strong non-Gaussian features such as intermittency and fat-tailed PDFs. The algorithms involve a hybrid strategy that requires only a small number of ensembles L. Here, a conditional Gaussian mixture in a high-dimensional subspace via an extremely e?cient parametric method is combined with a judicious Gaussian kernel density estimation in the remaining low-dimensional subspace. Then two effective strategies, a judicious block decomposition of the conditional covariance matrix and statistical symmetry, are developed and incorporated into these algorithms to deal with much higher dimensions even with orders in the millions and thus beat the curse of dimension. The algorithms are applied to a 1000-dimensional stochastic coupled FitzHugh-Nagumo model for excitable media. An accurate recovery of both the transient and equilibrium non-Gaussian PDFs requires only 1 sample! In addition, the block decomposition facilitates the algorithms to efficiently capture the non-Gaussian features at different locations in a 240-dimensional two-layer inhomogeneous Lorenz

96 model using only 500 samples.

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MS6

Closed-loop Reduced-order Control of Extreme Events in High-dimensional Systems

Rare events frequently occur in nonlinear and high-dimensional systems such as turbulent fluid flows and premixed flames. Due to their extreme nature, they can push engineering systems out of their operating envelope and reduce their lifetime. Here, we develop a control framework to suppress the occurence of these extreme events. Our approach is based on the Optimally Time-Dependent (OTD) modes, that have recently been used to formulate reliable indicators for the short-term prediction of rare events [Phys. Rev. E 94, 032212 (2016)]. First, we infer effective actuator locations from the spatial shape of the OTD modes, which align exponentially fast with the transiently most unstable subspace of the system. We then design an appropriate control law based on a reduced dynamical system obtained from the projection of the original system onto the OTD modes. We demonstrate the efficiency of the resulting control setup on relevant fluid dynamical examples.

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MS7

Sparsity in Low-rank Tensor Decompositions

Abstract not available at time of publication.

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MS7

Induced Distribution Sampling for Sparse Approximations

We present a new sampling scheme for computing sparse approximations to compressible polynomial chaos expansions. We first approximate the continuous distribution with a discrete set; this discrete set is constructed by sampling from the induced polynomial distribution. This construction ensures that, with a minimal number of samples and with high probability, the discrete set is a good emulator for the continuous distribution. This large sample set is subsequently sparsely subsampled, and function evaluations on this subsampled set are used in computing a sparse coefficient vector using weighted L1 optimization. The procedure is general, easily applicable to any tensor-product measure, and any polynomial index set. We show numerous examples illustrating the effectiveness of this algorithm in computing sparse approximations.

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MS7

Title Not Available

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MS7

Alternating Direction Method for Enhancing Sparsity of the Representation of Uncertainty

Compressive sensing has become a powerful addition to uncertainty quantification when only limited data is available. In this talk I will introduce a general framework to enhance the sparsity of the representation of uncertainty in the form of generalized polynomial chaos expansion. This framework uses an alternating direction method to identify new sets of random variables through iterative rotations such that the new representation of the uncertainty is sparser. Consequently, it increases both the efficiency and accuracy of the compressive sensing-based uncertainty quantification method. Numerical examples will be shown to demonstrate the effectiveness of this method.

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MS8

Using the Problem Symmetries to Improve Surrogates Models

Sometimes phenomena present symmetries, which allow us to obtain free information. We investigate multiphase cylindrical detonation in two-dimensions. We impose a trimodal perturbation in the particle volume fraction (PVF). We seek wave numbers that maximize the departure from axisymmetry at 500 ?s. We divide the domain into sectors in the azimuthal coordinate and we compute the difference of PVF in the sector with most particles and PVF in the sector with least particles. The amplitude for the three modes is the same and there is no phase shift, so the order of the wave-numbers does not matter. Hence for each combination of points we have 5 mirror points, i.e. the case with wave numbers (2,4,3) has mirror points (2,3,4) (3,2,4) (3,4,2) (4,2,3) (4,3,2). The symmetry helps to improve the surrogate model. Because our simulations are very expen-

sive we use multi-fidelity surrogates (MFS) to combine HF and low fidelity (LF) models to achieve accuracy at reasonable cost. The LF is obtained with coarser discretization achieving 85% cost savings. Two MFS were fitted: without using mirror points (70LF, 19HF) and using them (420LF, 114HF). The accuracy was measured using cross-validation error (CV), The inclusion of mirror points allowed a 46% reduction in CV error.

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MS8

Multi-fidelity Modeling for Optimizing Battery Design

We develop a new mathematical framework to study the optimal design of air electrode microstructures for lithium-oxygen (Li-O2) batteries. The design parameters to characterize an air-electrode microstructure include the porosity, surface-to-volume ratio, and parameters associated with the pore-size distribution. A surrogate model for discharge capacity is first constructed as a function of these design parameters. In particular, a Gaussian process regression method, co-kriging, is employed due to its accuracy and efficiency in predicting high-dimensional responses from a combination of multifidelity data. Specifically, a small sample of data from high-fidelity simulations are combined with a large sample of data obtained from computationally efficient low-fidelity simulations. The high-fidelity simulation is based on a multiscale modeling approach that couples the microscale (porescale) and macroscale (device-scale) models, while the low-fidelity simulation is based on an empirical macroscale model. The constructed response surface provides quantitative understanding and prediction about how air electrode microstructures affect the discharge capacity of Li-O2 batteries. The succeeding sensitivity analysis via Sobol indexes and optimization via genetic algorithm offer reliable guidance on the optimal design of air electrode microstructures. The proposed mathematical framework can be generalized to investigate other new energy storage techniques and materials.

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MS8

Linking Gaussian Process Regression with Data-driven Manifold Embeddings for Robust Nonlinear Information Fusion

In statistical modeling with Gaussian Process Regression, it has been shown that combining (few) high-fidelity data with (many) low-fidelity data enhances prediction accuracy, compared to prediction based on the few high-fidelity data only. Such information fusion techniques for multi-fidelity data commonly require strong cross-correlation between the high- and low-fidelity models. In real applications, however, cross-correlation across data at different fidelities may be obscured due to nonlinearity or multi-valuedness, resulting in degeneration of established techniques. Here, we present a robust mathematical algorithm for multiple fidelity information fusion that holds promise for alleviating the problem of hidden cross-correlations. We introduce higher-dimensional embeddings of the data, in which the high- and low-fidelity cross-correlations become more clear, and can be better exploited. The embedding theorems guarantee the one-to-oneness between the two data set embeddings. Then, the high-fidelity model turns into a function of the low-fidelity model on the appropriate manifold, which drastically enables established information fusion schemes. We describe the proposed framework and demonstrate its effectiveness through some benchmark problems, including models with discontinuities. The work establishes a useful synergy between theoretical concepts (observability, embedding theorems) and data-driven applications of machine learning.

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MS8

Deep Neural Networks for Multifidelity Uncertainty Quantification

A common scenario in computational science is the availability of a suite of simulators solving the same physical problem, such that the simulators are at varying levels of cost/fidelity. High fidelity simulators are more accurate but are computationally expensive, whereas low fidelity models can be evaluated cheaply while suffering from reduced accuracy. Additionally, many engineering applications are characterized by model parameters / boundary conditions / initial conditions etc. which are not known exactly. The surrogate-based approach to uncertainty quantification requires one to evaluate the forward model enough times such that one can construct a cheap (but accurate) approximation to the numerical solver. If the outputs from the simulators of varying fidelities are correlated, one can leverage information from low-fidelity simulators to augment information from a small number of evaluations of the high-fidelity simulator to construct an accurate surrogate model. In this work, we demonstrate a deep neural network (DNN) approach for constructing accurate surrogate models for uncertainty quantification by fusing information from multifidelity sources. DNNs are naturally suited for multifidelity information fusion because of the hierarchical representation of information. Our approach is validated on synthetic examples and demonstrated on real application examples from advanced manufacturing.

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MS9

Robust and Scalable Methods for the Dynamic

Mode Decomposition

The dynamic mode decomposition (DMD) is a low-rank approximation of time-series data which can be interpreted as the best fit linear dynamical system approximation of the data. Because of this interpretation, the DMD has applications in reduced order modeling and control. We consider the DMD from an algorithmic perspective and show that modern methods from the variable projection literature allow the DMD to be computed in a general setting. In particular, we show that the DMD can be computed in a manner which is robust to outliers in the data.

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MS9

Nonparametric Estimation for Stochastic Dynamical Systems

Given time series observations of a noisy system, how can we learn effective equations of motion? We frame this problem as nonparametric estimation of the drift f and diffusion Γ terms in systems of stochastic differential equations. We focus on models of the form $dX_t = f(X_t)dt + \Gamma dW_t$ where Γ is constant and W_t is Brownian motion. Given sufficiently high-frequency time series, we can directly attack the estimation problem using maximum likelihood techniques. This results in the same least-squares problem for the drift field f considered by Brunton, Proctor, and Kutz [PNAS, 2016]. When only low-frequency time series are available, we use diffusion bridge sampling to augment the data, leading to an expectation maximization (EM) algorithm. We study the performance of the EM approach as a function of signal-to-noise ratio, and compare EM against other techniques.

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MS9

Identifying Nonlinear Dynamics and Intrinsic Coordinates under Uncertainty

Abstract not available at time of publication.

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MS9

Sparse Identification of Nonlinear Dynamics for Model Predictive Control in the Low-data Limit

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MS10

UQ with Dependent Variables in Wind Farm Applications

One of the important aspects of UQ is the choice of input samples for complex (computationally expensive) simulations. For independent inputs, several well-known methods such as stochastic collocation exist. In case of dependent inputs for which only a dataset is available (while the underlying distribution is unknown), it is not clear how to adapt the existing methods from the independent case. We propose the use of partitioning and clustering methods to select the input samples and use an output approximation which is piecewise constant on the clusters. This leads to substantial improvement over Monte-Carlo sampling for strongly dependent datasets. Furthermore, we discuss a new method to find and quantify dependencies in large datasets. This method is based on estimating the Renyi entropy by minimum spanning trees (MSTs), including approximations to the MST for large datasets. The proposed method can be useful for sensitivity analysis. In this case, quantification of the dependencies between inputs and output leads to an ordering of the input variables, where the strongest dependency indicates that the corresponding input variable is most strongly affecting the output. With this goal in mind, a testcase is presented which applies these methods to the estimation of the power output of a wind turbine, given a dataset of weather conditions.

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MS10

Uncertainty Quantification in Large-scale Multiphysics Applications using Exascale Approaches

The study of complex physical systems is often based on computationally intensive high-fidelity simulations. To build confidence and improve the prediction accuracy of such simulations, the impact of uncertainties on the quantities of interest must be measured. This, however, requires a computational budget that is typically a large multiple of the cost of a single calculation, and thus may become unfeasible for expensive simulation models featuring a large number of uncertain inputs and highly non-linear behavior. In this regard, multi-fidelity methods have become increasingly popular in the last years as acceleration strategies to reduce the computational cost. These methods are based on hierarchies of generalized numerical resolutions or model fidelities, and attempt to leverage the correlation between high- and low-fidelity models to obtain a more accurate statistical estimator without requiring a large number of additional high-fidelity calculations. Exascale computing resources promise to facilitate the use of these approaches on larger scale problems by providing 1-10k times augmented floating-point capacity, but at expenses of requiring more complex data management as memory is expected to become more heterogeneous and distributed. The objective of this work, therefore, is to explore the performance of multi-fidelity strategies in large-scale multiphysics applications using Exascale-ready computational tools based on the Legion parallel programming system.

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MS10

An Efficient Reliability Analysis Tool for the Computation of Low Tail Probabilities and Extreme Quantiles in Multiple Failure Regions: Application to Organic Rankine Cycles

Calculation of tail probabilities is of fundamental importance in several domains, such as for example risk assessment. One major challenge consists in the computation of low-failure probability and multiple-failure regions, especially when an unbiased estimation of the error is required. Methods developed in literature rely mostly on the construction of an adaptive surrogate, tackling some problems such as the metamodel building criterion and the global computational cost, at the price of a generally biased estimation of the failure probability. In this study, we propose a novel algorithm permitting to both building an accurate metamodel and to provide a statistically consistent error. In fact, the proposed method provides a very accurate unbiased estimation even for low failure probability or multiple failure regions. Moreover, another importance sampling technique is proposed in this work, permitting to drastically reduce the computational cost when estimating some reference values, or when a very weak failure-probability event has to be computed directly from the metamodel. Several numerical examples are carried out, showing the very good performances of the proposed method with respect to the state-of-the-art in terms of accuracy and computational cost. The proposed method is finally applied to the reliability assessment of turbine cascades in Organic Rankine cycle flows.

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MS10

Closure Models for Quantifying Uncertainty in Multiphase Flow Transport Problems

Multi-phase flow prediction is of crucial importance in chemical processes, power plant and pipelines. Simulating multi-phase flow for realistic conditions is difficult, and simplifications are necessary to make computations tractable. A prominent example is the cross-sectional averaged one-dimensional two-fluid model (TFM), in which the effect of the smallest scales is captured via closure relations, like an interfacial friction model. However, the simplification introduced by averaging introduces a major issue, namely that the TFM becomes conditionally well-posed. This conditional well-posedness, and the uncertainties associated with closure relations, is a main open problem in the two-fluid model community. We take a new approach in solving the issue of well-posedness and closure relations in multi-phase flow. First, we perform high-fidelity (2D/3D) computations with two-phase flow CFD codes and use these to compute the unclosed quantities present in the 1D two-fluid model. Second, a neural network is trained that creates a functional relation between the averaged quantities and the closure terms. The neural network is built to include physical constraints, such as conservation law information, and trained under conditions for which the TFM is well-posed. Third, the trained model is evaluated and tested for conditions under which the conventional TFM is ill-posed, resulting in new physics-constrained closure models for multi-phase flow problems.

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MS11

Optimal Energy Storage Scheduling in Electricity Markets with Multiscale Uncertainty

We present a mathematical programming framework to study revenue opportunities for different classes of energy systems using historical wholesale market prices and physics-based models. For California markets, we show that up to 60% of revenue opportunities come from real-time markets, which requires strategic bidding to exploit price volatility. With this motivation, we compare different price forecasting methods for multiscale energy prices. An especially challenging aspect of energy markets is exploiting the wealth of data. For example, the California markets generated over 1 trillion unique spatial and time-varying price datum in 2015. For these reasons, we consider Gaussian Process Latent Variable Models to generate low-dimensional probabilistic forecasts to use as scenarios in stochastic programming formulations for bidding into energy markets.

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MS11

Uncertainty Quantification for Carbon Capture Systems

Uncertainty quantification (UQ) methods can help obtain reliable predictions for wide variety of carbon capture systems. Carbon capture systems are often represented by complex computational models and have many sources of uncertainty. These models often may be constrained to experimental data. Some of these sources of uncertainty include unknown model parameter values and physical constants, model form error, and experimental error. To explore these sources of uncertainty, a Bayesian calibration framework is often used; this calibration framework may include a model discrepancy term between the model and reality, and when necessary stochastic emulator trained to limited output from a computationally expensive model. This talk will discuss several advancements in UQ methodology for carbon capture systems as part of the Carbon Capture Simulation for Industry Impact ($CCSI^2$); calibration for solvent submodels, challenges with calibra-

tion/emulation for multi-scale models with a large number of parameters, upscaling uncertainty, and issues with experimental design.

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MS11

Estimating Uncertainities using Neural Network Surrogates and Dropout

Using machine learning has been shown to be a powerful means to explore, understand, and optimize the performance of inertial confine fusion (ICF) experiments. There is also a need to understand what are the uncertainty estimates in the predictions. Recent work has shown that large neural networks trained with the dropout regularization technique are approximations to a Gaussian process model. Using this technique we investigate the uncertainty in predictions for ICF simulations and determine how to best interpret the results of such predictions.

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MS11

Real-time Data Assimilation in Natural Gas Networks

We present a real-time data assimilation framework for large-scale natural gas networks. We demonstrate that the initial state is not observable given junction flow and pressure measurements in general but that the use of a steady-state prior is sufficient to infer the spatial fields of the networks during dynamic transients. We also demonstrate that, under a steady-state prior, junction pressure measurements are sufficient to infer the spatial fields. We also provide results using models of different physical resolution and demonstrate that these can be implemented rather easily using Plasmo.jl (a Julia-based graph-based modeling framework).

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MS12

Mathematical Modeling and Sampling of Stochastic Nonlinear Constitutive Laws on Smooth Manifolds

In this talk, we address the construction and sampling of high-dimensional stochastic models for spatially dependent anisotropic strain energy functions indexed by complex geometries. The models account for constraints related to convexity, coerciveness and consistency at small strains in the almost sure sense, hence making the representations mathematically consistent. The construction of an efficient sampling algorithm is subsequently proposed. The numerical strategy is based on solving a set of stochastic differential equations involving some underlying diffusion fields. The latter are specifically parametrized by local geometrical features inherited from the manifolds that define the boundaries of the domain under consideration. Various applications on vascular tissues are finally presented to demonstrate the relevance of the stochastic framework.

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MS12

Bayesian Uncertainty Quantification in the Prediction of Thermodynamical, Mechanical and Electronic Properties of Alloys using the Cluster Expansion Method

We present a framework for quantifying uncertainties when using the cluster expansion method as a surrogate model for quantum simulations in the prediction of material properties of alloys. Sparse Gaussian processes are used for simultaneous predictions in both the configuration space of alloys and temperature domain. We will show for the first time rigorous results in the calculation of phase diagrams of alloys with error bars induced by model error and epistemic uncertainty from training our models with limited data. Our approach has been used for several other temperature-dependent thermodynamic, mechanical and electronic properties including band structure and density of states (DOS).

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MS12

Stochastic Modeling of Multiscale Materials

Predictive modeling and design under uncertainty for complex systems can be achieved through a successful coupling of modeling tools, uncertainty quantification tools, and assimilation tools of available experimental data at a multitude of scales. Two challenges are associated with coupling these tools: 1) to characterize all available evidence in a probabilistic setting so as to capture key dependencies, and 2) to efficiently and accurately transform this evidence into inference concerning the design objective function. These challenges highlight the importance of accurate characterization of probabilistic priors and evaluations of likelihoods. Each of these steps is typically simplified for analytical and computational convenience. We present and demonstrate an approach for addressing these challenges for non-crimp fabric composites with minimum assumptions, by relying on polynomial chaos representations of both input parameters and multiscale material properties. These surrogates provide an accurate map from parameters (and their uncertainties) at all scales and the system-level behavior relevant for design. A key important feature of our proposed procedure is its efficiency and accuracy. It is a distinct approach to composite deign where the statistical dependence between the various material properties of the composites is not ignored, but rather introduced to impose mechanistic constraints on all the iterations within the design process.

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MS12

Identifying Sample Properties of Random Fields that Yield Response Maxima

We consider two types of stochastic inverse problems that arise from the mapping $A(x, Z) \mapsto U(x, Z)$ where $A(x, Z)$ is a random field, x is the spatial variable, Z is a random vector, and $U(x, Z)$ is the stochastic response. The first type is concerned with identifying the distribution of the random vector Z given probabilistic information of functionals of the response. The randomness in the response is due to the random field $A(x, Z)$ rather than observation noise, which may or may not be present. This type of inverse problems is ill-posed even if the inverse mapping is defined as point to set. We demonstrate through numerical examples and theoretical arguments the limitations of existing methods in obtaining meaningful solutions to this inverse problem. The second type of inverse problems assumes that the law of the random vector Z and all components of the mapping are fully specified. Our objective is to identify features of samples of the input random field $A(x, Z)$ which yield specified properties of response functionals, e.g., extremes of $U(x, Z)$ exceeding specified thresholds. We investigate this type of inverse problem using an example in mechanics and with the aid of surrogate models for the forward map.

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MS13

Active Subspaces in Parameterized Dynamical Systems

Defining, analyzing, and computing time-dependent active subspaces in dynamical systems. Implementing dynamic mode decomposition (DMD) [Schmid, 2010], sparse identification for nonlinear dynamical systems (SINDy) [Brunton et al., 2016], and other methods to discover and reconstruct dynamical systems that model global parameter sensitivity. Example applications include the Michaelis-Menten enzyme kinetics system, a 325-parameter combustion kinetics system, and the Lorenz system. This work provides unique insight into driving parameters in biological and engineering systems.

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MS13

The Underlying Connections Between Identifiability, Sloppiness, and Active Subspaces

Parameter space reduction and parameter estimation—and more generally, understanding the shape of the information contained in models with observational structure—are essential for many questions in mathematical modeling and uncertainty quantification. As such, different disciplines have developed methods in parallel for approaching the questions in their field. Many of these approaches, including identifiability, sloppiness, and active subspaces, use related ideas to address questions of parameter dimension reduction, parameter estimation, and robustness of inferences and quantities of interest. In this talk, we will discuss how active subspace methods have intrinsic connections to methods from sensitivity analysis and identifiability, and present a common framework for these approaches. A particular form of the Fisher information matrix (FIM), which we denote the sensitivity FIM, is fundamental to many of these methods. Through a series of examples and case studies, we illustrate the properties of the sensitivity FIM in several contexts. We illustrate how the interplay between local and global and linear and non-linear can affect these methods, and also show how borrowing tools from the other approaches can give new insights.

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MS13

Gauss–Christoffel Quadrature for Inverse Regression

Sufficient dimension reduction (SDR) provides a framework for reducing the predictor space dimension in regression problems. We consider SDR in the context of deterministic functions of several variables such as those arising in computer experiments. Here, SDR serves as a methodology for uncovering ridge structure in functions, and two primary algorithms for SDRsliced inverse regression (SIR) and sliced average variance estimation (SAVE)approximate matrices of integrals using a sliced mapping of the response. We interpret this sliced approach as a Riemann sum approximation of the particular integrals arising in each algorithm. We employ multivariate tensor product Gauss-Christoffel quadrature and orthogonal polynomials to produce new algorithms that improve upon the Riemann sum-based numerical integration in SIR and SAVE. We call the new algorithms Lanczos-Stieltjes inverse regression (LSIR) and Lanczos-Stieltjes average variance estimation (LSAVE) due to their connection with Stieltjes' method (and Lanczos' related discretization) for generating a sequence of polynomials that are orthogonal to a given measure. We show that the quadrature-based approach approximates the desired integrals, and we study the behavior of LSIR and LSAVE in numerical examples. As expected in high order numerical integration, the quadrature-based LSIR and LSAVE exhibit exponential convergence in the integral approximations compared to the first order convergence of the classical SIR and SAVE.

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MS13

Identifiability of Linear Compartmental Models:

The Singular Locus

Structural identifiability is the question of whether the parameters of a model can be recovered from perfect data. An important class of biological models is the class of linear compartmental models. Using standard differential algebra techniques, the question of whether a given model is generically locally identifiable is equivalent to asking whether the Jacobian matrix of a certain coefficient map, arising from the input-output equations, is generically full rank. A natural next step is to study the set of parameter values where the Jacobian matrix drops in rank, which we refer to as the locus of non-identifiable parameter values, or, for short, the singular locus. In this talk, we give a formula for these coefficient maps in terms of acyclic subgraphs of the model's underlying directed graph and study the case when the singular locus is defined by a single equation, the singular locus equation. In addition to giving a full understanding of the set of identifiable parameter values, we also show that the singular locus equation can be used to show certain submodels are generically locally identifiable. We determine the equation of the singular locus for two families of linear compartmental models, cycle and mammillary (star) models with input and output in a single compartment. We also state a conjecture for the corresponding equation for a third family: catenary (path) models.

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MS14

On the Interaction of Observation and Prior Error Correlations

The importance of prior error correlations in data assimilation has long been known, however, observation error correlations have typically been neglected. Recent progress has been made in estimating and accounting for observation error correlations, allowing for the optimal use of denser observations. Given this progress, it is now timely to ask how prior and observation error correlations interact and how this affects the value of the observations in the analysis. Addressing this question is essential to understanding the optimal design of future observation networks for high-resolution numerical weather prediction. The interaction of the prior and observation error correlations is illustrated with a series of 2-variable experiments in which the mapping between the state and observed variables (the observation operator) is allowed to vary. In an optimal system, the reduction in the analysis error variance and spread of information is shown to be greatest when the observation and prior errors have complementary statistics. This can be explained in terms of the relative uncertainty of the observations and prior on different spatial scales. It will be shown how the results from these simple 2-variable experiments can be used to inform the optimal observation density for higher dimensional problems.

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MS14

State Estimation for a Filtered Representation of a Chaotic Field

The numerical simulation of chaotic fields (e.g., turbulence, atmospheric convection, large-eddy simulation, wave-breaking, etc.) invariably leads to using a numerical grid (mesh) that is coarser than what is required to resolve all of the important physical processes being described by the set of governing partial differential equations. This coarse mesh will therefore miss important phenomena that the observational instruments used for state estimation will observe. We show here that the performance of state estimation can be improved by accounting for this fact that some physical processes are missing from the model simulations but observed by the observational instruments. We show how to properly construct a Bayesian framework for the situation where the numerical model is attempting to predict a truncated version of a much higher resolution state-vector and the observations that are being assimilated are observing the elements of this high-resolution state-vector. Then, we go on to describe a multi-resolution particle filtering framework that illustrates the main points of this theory as applied to a stochastic version of the Hénon Map.

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MS14

Feature Data Assimilation: A Tool for Model Tuning

Data-driven methods for extracting structures or features from a system of interest have been useful in many fields, including oceanography and geophysics, and in the study of dynamical systems. Correspondingly, the uses of these structures or features in data assimilation is of interest. A brief survey of feature data assimilation is presented, and the Bayesian formulation(s) of feature data assimilation are constructed. We then present several applications to model tuning, in which focusing on a particular feature in the data allows one to better tune model parameters to represent that feature.

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MS14

Addressing Uncertainty in Cloud Microphysics Using Radar Observations and Bayesian Methods

A leading-order source of error in numerical weather forecasts is the representation of clouds and precipitation, which is rife with uncertainties and approximations. This is, in part, an unavoidable consequence of the high degree of complexity inherent in modeling clouds and precipitation, as well as the lack of sufficiently detailed observa-

tions. However, much can still be done to quantify and constrain these uncertainties with the observations that do exist, such as widely available polarimetric weather radars. I will present research on three projects where Markov Chain Monte Carlo samplers are used to perform Bayesian estimation to gain microphysical information from radar observations. The first combines information on ice crystals from in situ cloud probes together with observations from two vertically-pointing radars, in order to improve understanding of the ice properties that influence large thunderstorm systems. The second is a Bayesian cloud property retrieval framework to leverage the information content of multi-frequency cloud radars. The third is a bulk microphysics parameterization scheme developed to eschew ad-hoc parameterization assumptions in favor of scheme structure and parameters that are entirely informed by radar observations themselves. An attendant advantage of our approach in all three projects is the robust (generally non-Gaussian and multivariate) estimate of uncertainty that is a reflection of our prior and observational uncertainties.

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MS15

Efficient Randomized Methods for D-Optimal Sensor Placement for Infinite-dimensional Bayesian Linear Inverse Problems Governed by PDEs

We address the problem of optimal experimental design (OED) for large-scale Bayesian linear inverse problems governed by PDEs. Specifically, the goal is to find optimal placement of sensors, where observational data are collected, so as to maximize the expected information gain. That is, we rely on the Bayesian D-optimal criterion given by the expected Kullback-Leibler divergence from posterior to prior. We introduce efficient randomized methods for fast computation of OED objective and its gradient, and rely on sparsifying penalty functions to enforce sparsity of the sensor placements. Numerical results illustrating our framework will be provided in the context of D-optimal sensor placement for optimal reconstruction of initial state in an advection-diffusion problem.

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MS15

Fast Methods for Bayesian Optimal Experimental Design

We cast data assimilation problem into a model inadequacy problem which is then solved by a Bayesian approach. The Bayesian posterior is then used for Bayesian Optimal Experimental Design (OED). Our focus is on the A- and D-optimal OED problems for which we construct scalable approximations that involve: 1) randomized trace estimators; 2) Gaussian quadratures; and 3) trace upper bounds. Unlike most of contemporary approaches, our methods work directly with the inverse of the posterior covariance, i.e. the Hessian of the regularized misfit for linear data assimilation problems, and hence avoiding inverting large matrices. We show that the efficiency of our methods can be further enhanced with randomized SVD. Various numerical results for linear inverse convection-diffusion data assimilation problems will be presented to validate our approaches.

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MS15

Optimal Positioning of Mobile Radiation Sensors Using Mutual Information

Locating and identifying a radiation source with information from stationary detectors is a well-documented inverse problem, but the optimal placement of such detectors is a more challenging task. In particular, optimal sensor placement depends on the location of the source, which is generally not known *a priori*. Mobile radiation sensors, which can adapt to the given problem, are an attractive alternative. While most mobile sensor strategies designate a trajectory for sensor movement, we instead employ mutual information to choose the next measurement location from a discrete set of design conditions. We use mutual information, based on Shannon entropy, to determine the measurement location that will give the most information about the source location and intensity.

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MS15

Sparse Sensor Placement in Bayesian Inverse Problems

We present a sparse optimization framework for the placement of measurement sensors in the sense of optimal design of experiments for infinite-dimensional Bayesian inverse problems . Here, the measurement setup is modelled by a regular Borel measure on the spatial domain. After

deriving an A-optimal design criterion, involving a sparse regularizer, we prove well-posedness of the problem and discuss first order optimality conditions . We present an approximation framework for the problem under consideration and discuss a priori estimates as well as the efficient numerical solution. The talk is concluded by numerical experiments.

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MS16

Convergence Properties of a Randomized Quasi-Newton Method for Least Squares Solutions to Linear Systems

Linear systems are pervasive throughout mathematics and the sciences. With the size of the systems we are solving outpacing the increase in computing power, new tools must be developed to solve problems in the regime of big data. We propose a randomized iterative quasi-Newton method which converges almost surely to the least squares solution of a linear system. Utilizing curvature information allows for faster descent but comes at the cost of inverting a high-dimensional Hessian. We show that preconditioning the data with a random matrix at each iteration allows the tradeoff between the rate of convergence and the cost per iteration to be favorable in terms of the time to convergence. We provide an uppper bound on the asymptotic rate of convergence and compare performance to that of more recognizable methods. We conclude with a discussion of future work: regularization, randomized dimension selection, and asynchronous parallelization.

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MS16

A Unifying Framework for Randomization Methods for Inverse Problems

We propose a unified approach for constructing scalable randomized methods for large-scale inverse problems. From this broader general framework, four different existing randomized methods for solving inverse problems (eNKF, RML, PCGA, and RMA) as well as new methods can be derived. This new unified theoretical understanding will help further the development and analysis of randomized methods for solving large-scale inverse problems. In particular, from our numerical comparisons and past work, we will demonstrate that misfit randomization methods lead to improved solutions compared to methods that randomize the prior part, and offer an intuition to support this idea.

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MS16

Subsampled Second Order Machine Learning and Scalable Quantification of Uncertainties

Abstract not available at time of publication.

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MS16

Low-Rank Independence Samplers for Bayesian Inverse Problems

In Bayesian inverse problems, the posterior distribution is used to quantify uncertainty about the reconstructed solution. MCMC algorithms often are used to draw samples from the posterior distribution; however, their implementations can be computationally expensive. We present a computationally efficient scheme for sampling high-dimensional Gaussian distributions in ill-posed Bayesian linear inverse problems. Our approach uses a proposal distribution based on a low-rank approximation of the prior-preconditioned Hessian. We show the dependence of the acceptance rate on the number of eigenvalues retained and discuss conditions under which the acceptance rate is high. Numerical experiments in image deblurring and computerized tomography show the benefits of our approach.

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MS17

Why Uncertainty Matters in Deterministic Computations: A Decision Theoretic Perspective

Probabilistic numerical methods have recently become an active area of research, for the purpose of quantifying epistemic uncertainty in deterministic computations, such as numerical integration, optimisation, numerical linear algebra and solutions for differential equations. Such uncertainty is caused by limited computational budges in solving

numerical tasks in practice, and arises as discretisation errors in approximating continuous objects. In the literature, several motivations have been given for such approaches, including propagation of uncertainties in a pipeline of numerical computations, aiming at the assessment of the resulting scientific conclusions, or at the optimal allocation of computational resources. In this talk, I will argue that another important motivation is provided by decision problems, where one is required to chose an optimal action from given candidate actions associated with possible losses. I will discuss how probabilistic numerical methods can play fundamental roles in such decision problems, showcasing several motivating examples.

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MS17

Compression, Inversion and Approximate Principal Component Analysis of Dense Kernel Matrices at Near-linear Computational Complexity

Many popular methods in machine learning, statistics, and uncertainty quantification rely on priors given by smooth Gaussian processes, like those obtained from the Matérn covariance functions. The resulting covariance matrices are typically dense, leading to (often prohibitive) $O\big(N^2\big)$ or $O\big(N^3\big)$ computational complexity.
In this work, we prove rigorously that the *dense* $N \times N$ kernel matrices obtained from elliptic boundary value problems and measurement points distributed approximately uniformly in a d-dimensional domain can be Cholesky factorised to accuracy ϵ in computational complexity $O\big(N \log^2(N) \log^{2d}(N/\epsilon)\big)$ in time and $O\big(N \log(N) \log^d(N/\epsilon)\big)$ in space. For the closely related Matérn covariances we observe very good results in practise, even for parameters corresponding to non-integer order equations. As a byproduct, we obtain a sparse PCA with near-optimal low-rank approximation property and a fast solver for elliptic PDE. We emphasise that our algorithm requires no analytic expression for the covariance function.
Our work connects the probabilistic interpretation of the Cholesky factorisation, the *screening effect* in spatial statistics, and numerical homogenisation. In particular, results from the game theoretic approach to numerical analysis ("Gamblets') allow us obtain rigorous error estimates.

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MS17

Boundary Value Problems: A Case Study for Nested Probabilistic Numerical Methods

Boundary value problems (BVPs) typically require two tools from numerical analysis: an approximation to the differential operator, as well as a nonlinear equation solver. Thus, BVPs are ideal candidates to study the interaction of numerical methods. Motivated by recent advances in probabilistic numerics, we propose to model the BVP solution with a Gaussian process and solve the nonlinear equation by iterations of Bayesian quadrature. The result is a probabilistic BVP solver that encapsulates the different sources of approximation uncertainty in its predictive posterior distribution. We test our method on a set of benchmark problems and indicate how Bayesian decision theory could use the probabilistic description to refine the solution.

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MS17

Probabilistic Implicit Methods for Initial Value Problems

Numerical integrators for IVPs that return probability measures instead of point estimates can be used to enrich the description of uncertainty in procedures requiring numerical computation of ODEs. An ever-expanding family of these methods are in development, within the recently emerging framework of Probabilistic Numerical Methods. One approach is to define a functional prior probability measure over the entire solution path, use time-stepping iterators to generate data, then output a functional posterior. Another approach, which allows for more interpretable analogues of classical algorithms, is based on randomising the integrator path at each step, aiming to match the error in the underlying method. This was introduced in Conrad et al. (2016), which provided an elegant convergence proof of the randomised method and discussed the complex issue of calibration. Teymur et al. (2016) considered an extension to Adams-type multistep methods and Lie et al (2017) provided some rigorous generalisations to the theory. This talk will briefly survey this approach, and discuss a new construction derived from implicit (multistep) integrators which boosts numerical stability.

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MS18

MCMC for High Energy X-Ray Radiography

Image deblurring via deconvolution can be formulated as a hierarchical Bayesian inverse problem, and numerically solved by Markov Chain Monte Carlo (MCMC) methods. Numerical solution is difficult because

- inconsistent assumptions about the data outside of the field of view of the image lead to artifacts near the boundary; and
- the Bayesian inverse problem is high-dimensional for high-resolution images.

The numerical MCMC framework I present addresses these issues. Boundary artifacts are reduced by reconstructing the image outside the field of view. Numerical difficulties that arise from high-dimensions are mitigated by exploiting sparse problem structure in the prior precision matrix.

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MS18

Iterative Construction of Gaussian Process Surrogate Models for Bayesian Inference in Combustion

A new algorithm is developed to tackle the issue of sampling non-Gaussian model parameter posterior probability distributions, which arise from solutions to Bayesian inverse problems characterized by expensive forward models. Gaussian process (GP) regression is utilized in constructing a surrogate model of the posterior distribution. An iterative approach is adopted for the optimal selection of points in parameter space used to train the GP surface. The efficacy of this new algorithm is tested on inferring reaction rate parameters in a hydrogen-oxygen combustion model.

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MS18

Rigorous Integration of Reduced-order Models in Bayesian Inference via Statistical Error Models

Performing Bayesian inference with large-scale models can be computationally costly due to the large number of forward solves incurred by posterior-sampling methods. To mitigate this cost, large-scale forward models are often replaced with an inexpensive surrogate model. Unfortunately, this strategy generally leads to incorrect posterior distributions, as the likelihood is incorrect: it does not reflect the error incurred by the surrogate model. This talk presents a strategy for reducing the computational cost of Bayesian inference while simultaneously improving the accuracy of the posterior by accounting for the error of the reduced surrogate model. The method (1) replaces the large-scale forward model with a projection-based reduced-order model, and (2) employs a statistical error model (constructed via the ROMES method) to quantify the discrepancy between the reduced-order model and the large-scale model. The resulting likelihood rigorously accounts for the epistemic uncertainty introduced by the reduced-order model, thereby enabling correct posteriors to be inferred, even when the reduced-order model itself is inaccurate.

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MS18

Data Assimilation with Stochastic Reduced Models

In weather and climate prediction, data assimilation combines data with dynamical models to make prediction, using ensembles of solutions to represent the uncertainty. Due to limited computational resources, reduced models are needed and coarse-grid models are often used, and the effects of the subgrid scales are left to be taken into account. A major challenge is to account for the memory effects due to coarse graining while capturing the key statistical-dynamical properties. We propose to use nonlinear autoregression moving average (NARMA) type models to account for the memory effects, and demonstrate by an example of the Lorenz 96 system that the resulting NARMA type stochastic reduced models can capture the key statistical and dynamical properties and therefore can improve the performance of ensemble prediction in data assimilation.

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MS19

A Sequential Sampling Strategy for Extreme Event Statistics in Nonlinear Dynamical Systems

We develop a method for the evaluation of extreme event statistics associated with nonlinear dynamical systems, using a very small number of samples. From an initial dataset of design points, we formulate a sequential strategy that provides the next-best data point (set of parameters) that when evaluated results in improved estimates of the probability density function (pdf) for a scalar quantity of interest. The approach utilizes Gaussian process regression to perform Bayesian inference on the parameter-to-observation map describing the quantity of interest. We then approximate the desired pdf along with uncertainty bounds utilizing the posterior distribution of the inferred map. The next-best design point is sequentially determined through an optimization procedure that selects the

point in parameter space that maximally reduces uncertainty between the estimated bounds of the pdf prediction. Since the optimization process utilizes only information from the inferred map it has minimal computational cost. Moreover, the special form of the criterion emphasizes the tails of the pdf. The method is applied to estimate the extreme event statistics for a very high-dimensional system with millions degrees of freedom: an offshore platform subjected to three-dimensional irregular waves. It is demonstrated that the developed approach can accurately determine the extreme event statistics using orders of magnitude smaller number of samples compared with traditional approaches.

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MS19

Predicting Statistical Response and Extreme Events in Uncertainty Quantification Through Reduced-order Models

The capability of using imperfect statistical and stochastic reduced-order models to capture crucial statistics in turbulent flow and passive tracers is investigated. Much simpler and more tractable block-diagonal models are proposed to approximate the complex and high-dimensional turbulent flow equations. The imperfect model prediction skill is improved through a judicious calibration of the model errors using leading order statistics. A systematic framework of correcting model errors with empirical information theory is introduced, and optimal model parameters under this unbiased information measure can be achieved in a training phase before the prediction. It is demonstrated that crucial principal statistical quantities in the most important large scales can be captured efficiently with accuracy using the reduced-order model in various dynamical regimes of the flow field with distinct statistical structures.

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MS19

Complementing Imperfect Models with Data for the Prediction of Extreme Events in Complex Systems

A major challenge in projection-based order reduction methods for nonlinear dynamical systems lies in choosing a set of modes that can faithfully represent the overall dynamics. Modes lacking in number or dynamical importance may lead to significant compromise in accuracy, or worse, completely different dynamical behaviors in the model. In this work, we present a framework for using data-driven models to assist dynamical models, obtained through projection, when the reduced set of modes are not necessarily optimal. We make use of the long short-term memory (LSTM), a recurrent neural network architecture, to extract latent information from the reduced-order time series data and derive dynamics not explicitly accounted for by the projection. We apply the framework to projected dynamical models of differing fidelities for prediction of intermittent events such as the Kolmogorov flow.

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MS20

Design of Optimal Experiments for Compressive Sampling of Polynomial Chaos Expansions

Polynomial chaos (PC) expansions are basis representations that are frequently used to construct surrogate models for complex problems, where model inputs are uncertain. Recently much work has been done regarding various input parameter sampling strategies for the purpose of constructing PC approximations. Further, concepts from the design of optimal experiments (DOE) have been applied to construct PC surrogates via compressed sensing or over determined least squares approximation. In general, optimal design are constructed by generating a large finite number of randomly generated candidate inputs then a subset of the candidate samples that optimizes a given object function is identified. While some research has been done to incorporate ideas from DOE to PC approximation, the role of sampling strategies used to generate candidate inputs has received less attention. In this work, we compare the performance of various sampling strategies used to generate candidate designs and the resulting effects those strategies have on the optimal designs constructed from the DOE and the quality of PC approximations.

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MS20

Sparse Approximation for Data-driven Polynomial Chaos Expansion and their Applications in UQ

In this talk, we will discuss collocation method via compressive sampling for recovering arbitrary Polynomial Chaos expansions (aPC). Our approach is motivated by the desire to use aPC to quantify uncertainty in models with random parameters. The aPC uses the statistical moments of the input random variables to establish the polynomial chaos expansion and can cope with arbitrary distributions with arbitrary probability measures. To identify the aPC expansion coefficients, we use the idea of Christoffel sparse approximation. We present theoretical analysis to motivate the algorithm. Numerical examples are also provided to show the efficiency of our method.

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MS20
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MS20
L1 Minimization Method for Link Flow Correction

A computational method, based on ℓ_1-minimization, is proposed for the problem of link flow correction, when the available traffic flow data on many links in a road network are inconsistent with respect to the flow conservation law. Without extra information, the problem is generally ill-posed when a large portion of the link sensors are unhealthy. It is possible, however, to correct the corrupted link flows accurately with the proposed method under a recoverability condition if there are only a few bad sensors which are located at certain links. We analytically identify the links that are robust to miscounts and relate them to the geometric structure of the traffic network by introducing the recoverability concept and an algorithm for computing it. The recoverability condition for corrupted links is simply the associated recoverability being greater than 1. In a more realistic setting, besides the unhealthy link sensors, small measurement noises may be present at the other sensors. Under the same recoverability condition, our method guarantees to give an estimated traffic flow fairly close to the ground-truth data and leads to a bound for the correction error. Both synthetic and real-world examples are provided to demonstrate the effectiveness of the proposed method.

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MS21
Uncertainty Quantification in High-dimensional Dynamical Systems Using a Data-driven Low-rank Approximation

We present a non-intrusive and data-driven method for constructing a low-rank approximation of high-dimensional stochastic dynamical systems. This method requires a snapshot sequence of samples of the stochastic field in the form of $\mathbf{A} \in \mathbb{R}^{n\times s\times m}$ where n is the number of observable data points, s is the number of samples and m is the number time steps. These samples may be generated using deterministic solvers or measurements. In this methodology, the time-dependent data is approximated by an r-dimensional reduction in the form of: $\mathbf{A}^r(t) = \mathbf{U}(t)\mathbf{Y}(t)^T$ where $\mathbf{U}(t) \in \mathbb{R}^{n\times r}$ is a set of deterministic time-dependent orthonormal basis and $\mathbf{Y}(t) \in \mathbb{R}^{s\times r}$ are the stochastic coefficients. We derive explicit evolution equations for $\mathbf{U}(t)$ and $\mathbf{Y}(t)$ and use the data to solve these equations. We demonstrate that this reduction technique captures the strongly transient stochastic responses with high-dimensional random dimensions. We demonstrate the capability of this method for time-dependent fluid mechanics problems.

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MS21
Warpings, Embeddings, and Latent Variables: The Quest of Learning from Multi-fidelity Data

The success of machine learning approaches to multi-fidelity modeling relies on their ability to distill useful cross-correlations between low- and high-fidelity data. Models based on linear auto-regressive schemes have yielded significant computational expediency gains on cases where such cross-correlations are predominately linear, however they fail to handle cases for which cross-correlations are complex. By identifying the capabilities and limitations of linear auto-regressive models, we propose a general framework for multi-fidelity modeling using deep neural networks. Motivated by the general embedding theorems of Nash, Takens, and Whitney, we demonstrate how nonlinear warpings, high-dimensional embeddings, and latent variables can help us disentangle factors of variation in the cross-correlation structure between low- and high-fidelity data. Finally, we put forth a collection of benchmark problems that and can help us analyze the advantages and limitations of existing algorithms, as well as highlight the effectiveness of the proposed approach.

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MS21
Hidden Physics Models: Machine Learning of Partial Differential Equations

While there is currently a lot of enthusiasm about "big data", useful data is usually "small" and expensive to acquire. In this paper, we present a new paradigm of learning partial differential equations from *small* data. In particular, we introduce *hidden physics models*, which are essentially data-efficient learning machines capable of leveraging the underlying laws of physics, expressed by time dependent and nonlinear partial differential equations, to extract patterns from high-dimensional data generated from experiments. The proposed methodology may be applied to the problem of learning, system identification, or data-driven discovery of partial differential equations. Our framework relies on Gaussian processes, a powerful tool for probabilistic inference over functions, that enables us to strike a balance between model complexity and data fitting. The effectiveness of the proposed approach is demonstrated through a variety of canonical problems, spanning a number of scientific domains, including the Navier-Stokes, Schrödinger, Kuramoto-Sivashinsky, and time dependent linear fractional equations. The methodology provides a promising new direction for harnessing the long-standing developments of classical methods in applied mathemat-

ics and mathematical physics to design learning machines with the ability to operate in complex domains without requiring large quantities of data.

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MS21

Physics-based Machine Learning via Adaptive Reduced Models and Multi-fidelity Modeling

New technologies are changing the way we think about designing and operating future engineering systems. In particular, the combination of sensing technologies and computational power brings new opportunities for data-driven modeling and data-driven decision-making. Yet data alone cannot deliver the levels of predictive confidence and modeling reliability demanded for safety-critical systems. For that, we must build on the decades of progress in rigorous physics-based modeling and associated uncertainty quantification. This talk discusses our work at the intersection of physics-based and data-driven modeling, with a focus on the design of next-generation aircraft. We show how adaptive reduced models combined with machine learning enable dynamic decision-making onboard a structural-condition-aware UAV. We show how multifidelity formulations exploit a rich set of information sources to achieve multidisciplinary design under uncertainty for future aircraft concepts.

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MS22

Control of Weakly Observed Nonlinear Dynamical Systems using Reinforcement Learning

Abstract not available at time of publication.

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MS22

An Information-theoretic Approach to Selecting Data-driven, Dynamical Systems via Sparse Regression

Abstract not available at time of publication.

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MS22

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MS23

Bayesian Inference for Estimating Discrepancy Functions in Rans Turbulence Model Closures

Due to their computational tractability, closure models within the Reynold-Averaged Navier-Stokes (RANS) framework remain a vital tool for modeling turbulent flows of engineering interest. However, it is well known that RANS predictions are locally corrupted by epistemic model-form uncertainty. A prime example of a modeling assumption with only a limited range of applicability is the Boussinesq hypothesis. We therefore aim to locally perturb the Boussinesq Reynolds stress tensor at locations in the flow domain where the modeling assumptions are likely to be invalid. However, inferring such perturbations at every location in the computational mesh leads to a high-dimensional inverse problem. To make the problem tractable, we propose two additional transport equations which perturb the shape of the modeled Reynolds stress tensor, such that the spatial structure is of the perturbation is pde-constrained. Exploring the posterior distribution of the Reynolds stresses (or other quantities of interest), can now be achieved through a low-dimensional Bayesian inference procedure on the coefficients of the perturbation model. We will demonstrate our framework on a range of flow problems where RANS models are prone to failure.

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MS23

Inference of Model Parameters in a Debris Flow Model Using Experimental Data

Calibration of complex fluid flow models from experimental data is not a straightforward problem, particularly when the data are difficult to interpret, incomplete or scarce, with the risk of reaching incorrect conclusions. This work tackles the problem of inferring in a Bayesian setting the

parameters of a complex non-linear debris-flow model from experimental data (see [D. L. George et al., Proceedings of the Royal Society of London A, 2014]). The data consist in time series of the debris flow thickness in a dam-break experiment. However, limited information is available regarding the processing and the precision of the data. Our Bayesian methodology constructs a surrogate model of the time series of debris flow elevation, using preconditioned polynomial chaos expansions, in order to reduce the computational effort to compute the MAP value of the parameters and sampling from the distribution. We contrast the results of the inference using the raw time series with the inference based on few selected features extracted from the original data. The comparison reveals that the idea of working on some important features is a relevant approach for this problem involving large modelling errors. Several reasons support this claim: the easier prescription of suitable and simpler likelihood definition; the computational complexity reduction; and the possibility of obtaining a better assessment of the posterior uncertainty by preventing over fitting of the parameters.

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MS23

Uncertainty Quantification Strategies in Systems of Solvers

The simulation of complex multi-physics phenomena often requires the use of coupled solvers, modelling different physics (fluids, structures, chemistry, etc) with largely differing computational complexities. We call Systems of Solvers (SoS) a set of interdependent solvers where the output of an upstream solver can be the input of a downstream solvers. A system of solvers typically encapsulate a large number of uncertain input parameters, challenging classical Uncertainty Quantification (UQ) methods such as spectral expansions and Gaussian process models which are affected by the curse of dimensionality. In this work, we develop an original mathematical framework, based on Gaussian Processes (GP) to construct a global metamodel of the uncertain SoS that can be used to solve forward and backward UQ problems. The key idea of the proposed approach is to determine a local GP model for each solver of the SoS. Several training strategies are possible from a priori training set generation and active learning methods that identify the most unreliable GP and proposes additional training points to improve the overall system prediction. The targeted systems of solvers are typically used to simulate complex multi physics flows. In particular, in this work, the methodology is applied to Space object reentry predictions.

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MS23

Comparison of Different Approximation Techniques for Uncertain Time Series Arising in Ocean Simulations

The analysis of time series is a fundamental task in many flow simulations such as oceanic and atmospheric flows. A major challenge is the construction of a faithful and accurate time-dependent surrogate with a manageable number of samples. Several techniques have been tested to handle the time-dependent aspects of the surrogate including a direct approach, low-rank decomposition, auto-regressive model and global Bayesian emulator. These techniques rely on two popular methods for uncertainty quantification, namely Polynomial chaos expansion and Gaussian processes regression. The different techniques were tested and compared on the uncertain evolution of the sea surface height forecast at two locations exhibiting different levels of variance. Two ensembles sizes were considered as well as two versions of polynomial chaos (ordinary least squares or ridge regression) and Gaussian processes (exponential or Matern covariance function) to assess their impact on the results. Our conclusions focus on the advantages and the drawbacks, in terms of accuracy, flexibility and computational costs of the different techniques.

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MS24

Risk-averse Optimal Power Flow via Surrogate Models

We present various numerical approaches for risk-adverse optimal power flow calculations based on stochastic surrogate modeling of power systems driven by renewable power sources. In our approaches, we minimize an averse risk measure of surrogate models of the generation cost. Such surrogates approximate the map between cost and random

and decision spaces. We propose two approaches for constructing cost surrogates: In the first approach we construct a basis expansion for the cost, with the coefficients estimated via sparse sampling from a limited set of random realizations of the system. In the second approach, we derive a quasi-Fokker-Planck equation, or probability density function (PDF) equation, for the state of the system. The stationary solution of the PDF equation is employed to approximate the PDF of the system's state, which is in turn used to estimate risk cost measures.

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MS24

Assimilating Data in Stochastic Dynamics

In this talk we introduce a statistical treatment of inverse problems with stochastic terms. Here the solution of the forward problem is given by a distribution represented numerically by an ensemble of simulations. We develop a strategy to solve such inverse problems by expressing the objective as finding the closest forward distribution that best explains the distribution of the observations in a certain metric. We propose to use metrics typically employed in forecast verification.

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MS24

Optimization and Design of Complex Engineering Systems using High-performance Computing

The optimization of many engineering systems reaches extreme size and unprecedented computational complexity due to the need to consider high fidelity physics and account for uncertainties. We will present scalable optimization algorithms and solvers for solving two such optimization problems: i. material optimization for the design of stiff structures using additive manufacturing; and, ii. economic optimization and control of large scale power grid systems under stochastic loads and generation. Our computational approach is based on scalable nonlinear programming algorithms, namely interior-point methods, and is specifically aimed at matching and surpassing the parallelism of existing physics solvers (e.g., finite element solvers for the elasticity problem governing material optimization) on massively parallel computing platforms. For this we developed specialized decomposition within the optimization, namely Schur complement-based decomposition for stochastic optimization and domain decomposition equipped with low-rank representations of the Hessian for material optimization. Finally, we present large scale simulations of the two motivating applications on the U.S. Department of Energy's supercomputers and provide a detailed discussion of the effectiveness and possible further improvement of the proposed techniques.

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MS24

PDF Estimation for Power Grid Systems via Sparse Regression

We present a numerical approach for approximating the probability density function (PDF) of quantities of interest (QoIs) of dynamical systems subject to uncertainty, with application to power grid systems driven by uncertain load and power generation. We employ Hermite polynomial expansions to construct a surrogate model for the map from random parameters to QoIs, which is then used to estimate the PDF of the QoIs via sampling. The coefficients of this expansion are estimated via compressed sensing from a small set of random realizations. The intrinsic low-dimensional structure of the map is exploited to identify a linear transformation of random space via iterative rotations that enhances the sparsity of the Hermite representation. The proposed sparse sampling approach requires significantly less realizations of the full dynamics of the system than the standard least squares method to construct the surrogate model. The PDF estimates provided by our approach are more accurate in terms of the Kullback-Leibler divergence than Monte Carlo estimates while using fewer realizations.

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MS25

Stochastic Modeling of Uncertainties in Fast Essential Antarctic Ice Sheet Model

Quantifying the uncertainty in projections of sea-level rise induced by ice-sheet dynamics is a pivotal problem in assessing climate-change consequences. Sources of uncertainty in ice-sheet models include uncertain climate forcing, basal friction, sub-shelf melting, initialization, and other model features. Accounting for uncertainty in ice-sheet models (ISMs) is challenging: (i) the stochastic modeling of sources of uncertainty can be challenged by data scarcity and imperfect representations of physical processes, and (ii) the computational cost of ISMs can hinder their integration in Earth system models and limit the number of simulations available for uncertainty propagation. In

this talk, we address the uncertainty quantification of sea-level rise projections by using the new fast essential ISM f.ETISh that affords computational tractability by limiting its complexity to the essential interactions and feedback mechanisms of ice-sheet flow. After highlighting how simulations require an initialization procedure that precedes their use in predicting climate-change effects, we will discuss the sources of uncertainty in this ISM and the information available for their stochastic modeling. We will show the stochastic modeling of a subset of these sources of uncertainty, followed by a propagation of uncertainty through the ISM and a sensitivity analysis to help identify the dominant sources of uncertainty in sea-level rise projections.

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MS25

On the Robustness of Variational Multiscale Error Estimators for the Forward Propagation of Uncertainty

In this talk, we focus on the definition of a family of deterministic error estimators to characterize the discretization error for uncertainty quantification purposes. We first address the construction of a posteriori error estimators based on the Variational Multiscale (VMS) method with orthogonal subscales for the convection-diffusion-reaction (CDR) problem. Here, the global error estimator (rather than the distribution of the local error over the domain) is selected as the quantity of interest. The behavior of the error estimator is subsequently characterized introducing system-parameter uncertainties in the coefficients of the CDR problem. The propagation of these uncertainties is conducted using a polynomial chaos expansion and a projection method, and convergence with respect to mesh refinement is finally investigated.

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MS25

Coarse Approximation of Highly Oscillatory Random Elliptic Problems

We consider an elliptic problem with highly oscillatory, possibly random coefficients. We show how to approximate it using a problem of the same type, but with constant and deterministic coefficients, that are defined by an optimization procedure. The approach is robust to the fact that the information on the oscillatory coefficients in the equation can be incomplete. In the limit of infinitely small oscillations of the coefficients, we illustrate the links between this approach and the classical theory of homogenization, based on solving corrector problems. Comprehensive numerical tests and comparisons will be discussed, that show the potential practical interest of the approach. This is joint work with Claude Le Bris (Ecole des Ponts and Inria) and Simon Lemaire. Reference: https://arxiv.org/abs/1612.05807

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MS25

Surrogate-based Bayesian Inversion for the Model Calibration of Fire Insulation Panels

We outline an approach for the calibration of a finite element model (FEM), describing the heat transfer in insulation when exposed to fire, by using a full Bayesian inference approach. The considered FEM uses so-called *temperature dependent effective material parameters*. These parameters are required for applying the *improved component additive method* to determine the fire resistance of e.g. timber frame assemblies. We herein propose a full Bayesian procedure, that allows the sought model parameters to be calibrated in an efficient way. We distinguish two approaches, namely (1) a standard Bayesian parameter estimation approach and (2) a more involved hierarchical Bayesian modeling approach. The standard Bayesian approach is applicable to the case of single measurements, where a best fit considering measurement and modeling errors is sought. The hierarchical approach can be applied to cases where multiple measurements under differing experimental conditions are available, so as to capture the variability of effective material parameters across experiments. Bayesian inference is typically carried out using computationally expensive Markov Chain Monte Carlo (MCMC) simulations. To circumvent these limitations, we use a surrogate modeling technique (polynomial chaos expansion). This surrogate model can be used in MCMC simulations instead of the actual forward model and helps reducing the computational burden to a feasible level.

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MS26

Inherent Limitations to Parameter Estimation in Cancer Incidence Data

Multistage clonal expansion models are used to tie cancer incidence data to the modeled underlying biological processes of carcinogenesis. Characterizing the amount and form of the information available in cancer incidence data for this class of models is vitally important for understanding the implications of parameter estimates for the underlying biology and for predictions of future cancer incidence rates. We use profile likelihood methods from practical identifiability analysis to show that the usual cancer incidence data has inherently less information than theoretical structural identifiability analysis suggests, allowing us to systematically reduce the dimension of the estimated pa-

rameter space.

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MS26

Structural Identifiability Analysis of Matrix Models for Structured Populations

Matrix models are commonly used in ecology and natural resource management, where they provide suitable modeling frameworks for age and stage structured populations. In this talk, we will examine how the model parameterization affects behavior and parameter estimation using identifiability and sensitivity analysis methods. We use both structural and practical identifiability analysis to examine which parameters can be estimated uniquely from data. We then use a combination of local and global sensitivity analysis to evaluate which parameters are strong potential intervention targets. The methods developed for examining the matrix models considered here can also be generalized to a range of matrix and difference equation models.

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MS26

Parameter Identifiability and Effective Theories in Physics, Biology, and Beyond

The success of science is due in large part to the hierarchical nature of physical theories. These effective theories model natural phenomena as if the physics at macroscopic length scales were almost independent of the underlying, shorter-length-scale details. The efficacy of these simplified models can be understood in terms of parameter identifiability. Parameters associated with microscopic degrees of freedom are usually unidentifiable as quantified by the Fisher Information Matrix. I apply an information geometric approach in which a microscopic, mechanistic model is interpreted as a manifold of predictions in data space. Model manifolds are often characterized by a hierarchy of boundaries–faces, edges, corners, hyper-corners, etc. These boundaries correspond to reduced-order models, leading to a model reduction technique known as the Manifold Boundary Approximation Method. In this way, effective models can be systematically derived from microscopic first principles for a variety of complex systems in physics, biology, and other fields.

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MS27

Adaptive Meshfree Backward SDE Filter

An adaptive meshfree approach is proposed to solve the nonlinear filtering problem based on forward backward stochastic differential equations. The algorithm relies on the fact that the solution of the forward backward stochastic differential equations is the unnormalized filtering density as required in the nonlinear filtering problem. Adaptive space points are constructed in a stochastic manner to improve the efficiency of the algorithm. We also introduce a Markov chain Monte Carlo resampling method to address the degeneracy problem of the adaptive space points. Numerical experiments are carried out against the auxiliary particle filter method in the rugged double well potential problem as well as the multi-target tracking problem to demonstrate the superior performance of our algorithm.

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MS27

Multilevel Picard Approximations for High-dimensional Nonlinear Parabolic Partial Differential Equations and High-dimensional Nonlinear Backward Stochastic Differential Equations

We introduce, for the first time, a family of algorithms for solving general high-dimensional nonlinear parabolic partial differential equations with a polynomial complexity in both the dimensionality and the reciprocal of the accuracy requirement. The algorithm is obtained through a delicate combination of the Feynman-Kac and the Bismut-Elworthy-Li formulas, and an approximate decomposition of the Picard fixed- point iteration with multi-level accuracy. The algorithm has been tested on a variety of nonlinear partial differential equations that arise in physics and finance, with very satisfactory results. Analytical tools needed for the analysis of such algorithms, including a nonlinear Feynman-Kac formula, a new class of seminorms and their recursive inequalities, are also introduced. They allow us to prove that for semi-linear heat equations, the computational complexity of the proposed algorithm is bounded by $O(d * \varepsilon^{-4})$ for any $d > 0$, where d is the dimensionality of the problem and $\varepsilon \in (0, 1)$ is the prescribed accuracy.

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MS27

Deep Optimal Stopping: Solving High-dimensional Optimal Stopping Problems with Deep Learning

Optimal stopping problems suffer from the curse of dimensionality. This talk concerns a new deep learning method for solving high-dimensional optimal stopping problems. In particular, the introduced algorithm can be employed for solving optimal equipment replacement problems and for the pricing of American options with a large number of

underlyings. The presented algorithm is in fact applicable to a very broad class of financial derivatives (such as path-dependent American, Bermudan, and Asian options) as well as multifactor underlying models (such as Heston-type stochastic volatility models, local volatility models, and jump-diffusion models). Moreover, the algorithm allows to approximatively compute both the price as well as an optimal exercise strategy for the American option claim. Numerical results on benchmark problems are presented which suggest that the proposed algorithm is highly effective in the case of many underlyings, in terms of both accuracy and speed.

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MS27

Bayesian Inference via Filtering Equations for Financial Ultra-high Frequency Data

We propose a general partially-observed framework of Markov processes with marked point process observations for ultra-high frequency (UHF) transaction price data, allowing other observable economic or market factors. We develop the corresponding Bayesian inference via filtering equations to quantify parameter and model uncertainty. Specifically, we derive filtering equations to characterize the evolution of the statistical foundation such as likelihoods, posteriors, Bayes factors and posterior model probabilities. Given the computational challenge, we provide a convergence theorem, enabling us to employ the Markov chain approximation method to construct consistent, easily-parallelizable, recursive algorithms. The algorithms calculate the fundamental statistical characteristics and are capable of implementing the Bayesian inference in real-time for streaming UHF data, via parallel computing for sophisticated models. The general theory is illustrated by specific models built for U.S. Treasury Notes transactions data from GovPX and by Heston stochastic volatility model for stock transactions data.

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MS28

Sobol' Indices for Sensitivity Analysis with Dependent Inputs

When performing global sensitivity analysis (GSA), it is often assumed, for the sake of simplicity, for lack of information or for sheer expediency, that uncertain variables in the model are independent. It is intuitively clear-and easily confirmed through simple examples-that applying a GSA method designed for independent variables to a set of correlated variables generally leads to results that hard to interpret, at best. We generalize the probabilistic framework for GSA pioneered by Sobol' to problems with correlated variables; this is done by reformulating his indices in terms of approximation errors rather than variance analysis. The implementation of the approach and its computational complexity are discussed and illustrated on synthetic examples.

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MS28

Global Sensitivity Analysis of Models with Dependent and Independent Inputs

Global sensitivity analysis (GSA) is used to identify key parameters whose uncertainty most affects the model output. This information can be used to rank variables, fix or eliminate unessential variables and thus decrease problem dimensionality. Variance-based Sobol sensitivity indices (SI) are most frequently used in practice owing to their efficiency and ease of interpretation. Most existing techniques for GSA were designed for models with independent inputs. In many cases, there are dependencies among inputs, which may have a significant impact on the results. Such dependences in a form of correlations have been considered in our previous works. There is a wide class of models involving inequality constraints which impose structural dependencies between model variables. In this case, the parameter space may assume any shape depending on the number and nature of constraints. This class of problems encompasses a wide range of situations encountered in the natural sciences, engineering, economics, etc, where model variables are subject to certain limitations imposed e.g. by conservation laws, geometry, costs etc. In this talk, we consider two approaches for estimating Sobol SI for constraint GSA. The classical one is based on using direct integral formulas. In the second approach, a metamodel of the original full model is constructed first and then this metamodel is used for estimating Sobol SI. This approach significantly reduces the cost of evaluation Sobol SI.

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MS28

Goal-oriented Sensitivity Analysis Using Perturbed-law Based Indices

One of the most critical hypothesis in uncertainty propagation studies is the choice of the distributions of uncertain input variables which are propagated through a computational model. In general, such probability distributions come from various sources : statistical inference, design or operation rules, expert judgment, etc. In all cases, the probabilistic models for these variables are established with a certain level of accuracy or confidence. Hence, bringing stringent justifications to the overall approach requires quantifying the impact of the assumptions made on the input laws on the output criterion. Perturbed Law based Indices (PLI) perform such a robustness analysis, different from the standard sensitivity analysis methods. The principle is to assess the influence of a perturbation on a parameter or a moment of the input distribution, on some output quantity of interest. Any quantity of interest can be considered, as the mean of the model output, its variance, a probability that the output exceeds a threshold or a quantile of the output.

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MS28

Shapley Effects for Sensitivity Analysis with Dependent Inputs

Global sensitivity analysis of a numerical model consists in quantifying, by the way of sensitivity indices, the contributions of each of its input variables in the variability of its output. Based on the functional variance analysis, the popular Sobol indices present a difficult interpretation in the presence of statistical dependence between inputs. Recently introduced, the Shapley effects, which consist of allocating a part of the variance of the output at each input, are promising to solve this problem. In this talk, from several analytical results, we study the effects of linear correlation between some Gaussian input variables on Shapley effects, comparing them to classical first-order and total Sobol indices. This illustrates the interest, in terms of interpretation, of the Shapley effects in the case of dependent inputs. We also empirically study the numerical convergence of estimating the Shapley effects. For the engineering practical issue of computationally expensive models, we show that the substitution of the model by a metamodel makes it possible to estimate these indices with precision. The results presented during that talk include joint work with Art Owen (Stanford University, USA) and Bertrand Iooss (EDF, Paris, France).

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MS29

High-dimensional Stochastic Inversion via Adjoint Models and Machine Learning

Performing stochastic inversion on a computationally expensive forward simulation model with a high-dimensional uncertain parameter space (e.g. a spatial random field) is computationally prohibitive even with gradient information provided. Moreover, the 'nonlinear' mapping from parameters to observables generally gives rise to non-Gaussian posteriors even with Gaussian priors, thus hampering the use of efficient inversion algorithms designed for models with Gaussian assumptions. In this paper, we propose a novel Bayesian stochastic inversion methodology, characterized by a tight coupling between a gradient-based Langevin Markov Chain Monte Carlo (LMCMC) method and a kernel principal component analysis (KPCA). This approach addresses the 'curse-of-dimensionality' via KPCA to identify a low-dimensional feature space within the highdimensional and nonlinearly correlated spatial random field. Moreover, non-Gaussian full posterior probability distribution functions are estimated via an efficient LMCMC method on both the projected lowdimensional feature space and the recovered high-dimensional parameter space. We demonstrate this computational framework by integrating and adapting recent developments such as data-driven statistics-on-manifolds constructions and reduction-through-projection techniques to solve inverse problems in linear elasticity.

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MS29

An Iterative Local Updating Ensemble Smoother for High-dimensional Inverse Modeling with Multimodal Distributions

Ensemble smoother (ES) has been widely used in high-dimensional inverse modeling. However, its application is limited to problems where uncertain parameters approximately follow Gaussian distributions. For problems with multimodal distributions, using ES directly would be problematic. One solution is to use a clustering algorithm to identify each mode, which is not very efficient when the dimension is high or the number of modes is large. Alternatively, we propose in this paper a very simple and efficient algorithm, i.e., the iterative local updating ensemble smoother (ILUES), to explore multimodal distributions in high-dimensional problems. This algorithm is based on updating local ensembles of each sample in ES to explore possible multimodal distributions. To achieve satisfactory data matches in nonlinear problems, we adopt an iterative form of ES to assimilate the measurement multiple times. Five numerical case studies are tested to show the performance of the proposed method. To show its applicability in practical problems, we test the ILUES algorithm with three inverse problems in hydrological modeling that have multimodal prior distribution, multimodal posterior distribution and a large number of unknown parameters, respectively.

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MS29

Using Surrogate Models to Accelerate Bayesian Inverse UQ

The laser flash experiment is a wellknown technique used to determine the unknown thermal diffusivity of a material. The temperature of a material specimen is measured using an infrared sensor at discrete times over a time interval containing a heating laser flash. The temperature of the specimen is modelled as the solution of a timedependent partial differential equation (PDE). As their actual values are unknown, some parameters of the PDE are modelled as random variables. Such parameters include the coefficients (including the thermal diffusivity) and boundary conditions. We pose the problem of estimating the thermal diffusivity as a Bayesian inverse problem, aiming to approximate the posterior distribution, given experimental data obtained from a laser flash experiment. Markov chain Monte Carlo (MCMC) sampling algorithms require calculation of the posterior density at each iteration. Here, each evaluation of the posterior requires the timedependent PDE to be solved numerically. This results in an incredibly computationally expensive routine, taking days to produce enough samples to approximate the posterior sufficiently well. We use a surrogate model within an MCMC routine to reduce this cost. Specifically, we use a stochastic Galerkin FEM solution to the PDE as a surrogate for repeatedly computing deterministic FE solutions. Investigations into how both the speed and accuracy of the approximation of the posterior are affected by this replacement are presented.

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MS29

Learning Physical Laws from Noisy Data

We present a new data-driven approach to learn ordinary and partial differential equations, particularly, shallow water equations and Navier-Stokes equations. The key idea is to identify the terms in the underlying fluid equations and to approximate the weights of terms with error bars using Bayesian machine learning algorithms. In particular, Bayesian sparse feature selection and parameter estimation are performed. Numerical experiments show the robustness of the learning algorithms with respect to noisy data and its ability to learn various candidate equations with error bars to represent the quantified uncertainty. Also, comparisons with sequential threshold least squares and lasso are studied from noisy measurements. Prediction with error bars using our algorithm is illustrated at the end.

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MS30

Bridging High Performance Computing for Experimental Neutron Sciences

This talk will focus on mathematics developed to help bridge the computational and experimental facilities at Oak Ridge National Laboratory (ORNL). This talk will demonstrate that sparse sampling methods for large scale experimental data can utilize HPC to analyze data for experimental neutron sciences. Sparse sampling has the ability to provide accurate reconstructions of data and images when only partial information is available for measurement. Sparse sampling methods have demonstrated to be robust to measurement error. These methods have the potential to scale to large computational machines and analysis large volumes of data.

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MS30

Efficient Numerical Methods for Stochastic Schrodinger Equations

We study SIMPLEC algorithm for stochastic Schrodinger equations.

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MS30

Accounting for Model Error from Unresolved Scales in Ensemble Kalman Filters by Stochastic Parameterization

In this talk, the use of discrete-time stochastic parameterization will be investigated by numerical experiments to account for model error due to unresolved scales in ensemble Kalman filters. The parameterization produces an improved non-Markovian forecast model, which generates

high quality forecast ensembles and improves filter performance. Results are compared with the methods of dealing with model error through covariance inflation and localization (IL), using as an example the two-layer Lorenz-96 system.

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MS30

A Probabilistic Analysis and Rare Event Study of a Dynamical Queue for Modeling Human Operators

We study a model for task management for human operators. A novel approach to modeling the system is by considering a dynamical queue, in which a dynamical quantity called the utilization ratio tracks the approximate stress level an operator experiences while working. The case when the service time of a task entering service is a deterministic function of the utilization ratio has been well studied. The function was found, via experimental studies, to follow a Yerkes-Dodson law, a principle from psychology where human operators work more efficiently with more stress up to a point, where further increases in stress will decrease the effective work rate. We introduce a probabilistic version of the queue, where the service time is conditionally distributed on the value of the Yerkes-Dodson law and the utilization ratio. We analyze the behavior of the probabilistic dynamical queue when the service time distribution is conditionally exponential via the method of supplementary variables. We find its Chapman-Kolmogorov equations and study its stationary distribution. We also study general service time distributions via simulation. Rare events, such as the probability of buffer overflow, are also considered. Methodology adapted to this problem include perfect simulation via coupling from the past. Importance sampling and splitting methods based on large deviations are used to study rare events. Improvements to rare event simulation is considered with use with transport maps.

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MS31

A Scalable Design of Experiments Framework for Optimal Sensor Placement

We present the design of experiments framework for sensor placement in the context of state estimation of natural gas networks. We aim to compute optimal sensor locations where observational data are collected, by minimizing the uncertainty in parameters estimated from Bayesian inverse problems, which are governed by partial differential equations. The resulting problem is a mixed-integer nonlinear program. We approach it with two recent heuristics that have the potential to be scalable for such problems: a sparsity-inducing approach and a sum-up rounding approach. We investigate two objectives: the total flow variance and the A-optimal design criterion. We conclude that the sum-up rounding approach produces shrinking gaps with increased meshes. We also observe that convergence for white noise measurement error is slower than for the colored noise case. For the A-optimal design, the solution is close to the uniform distribution, but for the total flow variance the pattern is noticeably different.

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MS31

Accelerated MCMC using Bayesian Optimization

Markov Chain Monte Carlo (MCMC) has become the main computational workhorse in scientific computing for solving statistical inverse problems. It is difficult however to use MCMC algorithms when the likelihood function is computationally expensive to evaluate. The status quo tackles this problem by emulating the computationally models upfront based on a number of forward simulations, and then the emulator is used in the MCMC simulation instead of the actual model. However, this strategy has an obvious drawback: how should one choose the initial number of forward simulations to capture the complexity of the model response? A novel Metropolis-Hastings algorithm is proposed to sample from posterior distributions corresponding to computationally expensive simulations. The main innovation is emulating the likelihood function using Gaussian processes. The proposed emulator is constructed on the fly as the MCMC simulation evolves and adapted based on the uncertainty in the acceptance rate. The algorithm is tested on a number of benchmark problems where it is shown that it significantly reduces the number of forward simulations.

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MS31

Leader Selection in Stochastically Forced Consensus Network

We are interested in assigning a pre-specified number of nodes as leaders in order to minimize the mean-square deviation from consensus in stochastically forced networks.

This problem arises in several applications including control of vehicular formations and localization in sensor networks. For networks with leaders subject to noise, we show that the Boolean constraints (a node is either a leader or it is not) are the only source of nonconvexity. By relaxing these constraints to their convex hull we obtain a lower bound on the global optimal value. We also use a simple but efficient greedy algorithm to identify leaders and to compute an upper bound. For networks with leaders that perfectly follow their desired trajectories, we identify an additional source of nonconvexity in the form of a rank constraint. Removal of the rank constraint and relaxation of the Boolean constraints yields a semidefinite program for which we develop a customized algorithm well-suited for large networks. Several examples ranging from regular lattices to random graphs are provided to illustrate the effectiveness of the developed algorithms.

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MS31

Optimal Experimental Design for Metallic Fatigue Data

The optimal planning of follow-up experiments requires the specification of a model of interest and the application of efficient computational methods for the exploration of the design space. In this talk, we introduce a design problem that arises from the information gathered from fatigue tests performed at the Battelle Memorial Institute upon unnotched sheet specimens of 75S-T6 aluminum alloys. For a comprehensive statistical analysis of the original fatigue dataset, the calibration of some proposed models to deal with right-censored data and the treatment of model comparison, see Babuška, I. et al., Bayesian inference and model comparison for metallic fatigue data, Comput. Methods Appl. Mech. Engrg. 304 (2016) 171-196. Under a Bayesian framework, given some selected models, we apply different computational techniques for the estimation of the expected information gain to determine optimal follow-up experiments.

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MS32

Bayesian Quadrature for Multiple Related Integrals

Bayesian probabilistic numerical methods are a set of tools providing posterior distributions on the output of numerical methods. The use of these methods is usually motivated by the fact that they can represent our uncertainty due to incomplete/finite information about the continuous mathematical problem being approximated. In this talk, we demonstrate that this paradigm can provide additional advantages, such as the possibility of transferring information between several numerical methods. This allows users to represent uncertainty in a more faithfully manner and, as a by-product, provide increased numerical efficiency. We propose the first such numerical method by extending the well-known Bayesian quadrature algorithm to the case where we are interested in computing the integral of several related functions. We then demonstrate its efficiency in the context of multi-fidelity models for complex engineering systems, as well as a problem of global illumination in computer graphics.

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MS32

Adaptive Bayesian Quadrature for Approximate Inference

Bayesian Quadrature (BQ) is a is a rigorous framework for constructing posterior measures over integrals $F = \int f(x)\,dx$ and allows for the incorporation of explicit priors, active selection of evaluation nodes, as well as a sound treatment of uncertainty. Despite its algebraic beauty, BQ has found little practical use in machine learning. Computational cost cubic in the number of evaluation nodes countervails their spatial coverage and prevents GP-based BQ from scaling to high-dimensional tasks. To achieve competitiveness with state-of-the-art MCMC, the BQ prior has to be tailored to the specific integration task. We focus on approximate inference as field of application, which involves the computation of a potentially high-dimensional integral, the evidence. In this setting, speed-up compared to vanilla BQ can be achieved by specifically modeling a positive integrand and by evaluating the integrand in an adaptive manner in order to discover high-mass regions. I will report on strategies as well as challenges in making BQ practicable even for high-dimensional integration problems.

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MS32

Adaptive Bayesian Cubature using Quasi-Monte Carlo Sequences

Multidimensional integrals are often evaluated by simple Monte Carlo methods. Quasi-Monte Carlo methods employ correlated sequences whose empirical distribution function better mimics the distribution defining the integral. The author and his collaborators have recently developed methods for adaptively determining the sample size, n, of (quasi-)Monte Carlo methods needed to satisfy the user's error requirements. This talk describes an approach where the integrand is assumed to arise from a Gaussian process. Because quasi-Monte Carlo sequences and their matching kernels are used, the computational cost is $O(n \log n)$, rather than the typical $O(n^3)$ required to determine the cubature weights and estimate the the parameters in the covariance kernel. The credible interval is used to determine the number of data sites required to meet the predetermined error tolerance. We provide numerical examples.

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MS32

Fully Symmetric Sets for Efficient Large-Scale Probabilistic Integration

Kernel-based approximation methods typically suffer from the characteristic cubic computational and quadratic space

complexity in the number of data points, hindering their use in many applications where a lot of data is required. We show that kernel (or Bayesian) quadrature rules, that carry a probabilistic interpretation allowing for meaningful quantification of uncertainty inherent to integral approximations, can be constructed efficiently for up to millions of points and in high dimensions if the node set is a union of fully symmetric sets, each such set consisting of all coordinate permutations and sign changes of a given vector. The central observation permitting (under some rather lax assumptions on symmetricity of the kernel and the integration measure) fast and exact computation of kernel quadrature weights is that all nodes in one fully symmetric set share the same weight. Consequently, the number of distinct weights that need to be computed is greatly diminished. For selecting the fully symmetric sets we propose a few different schemes, the most promising of these being sparse grids. The main drawback of the method is that we are not able to extend it beyond computing the quadrature weights. In particular, principled fitting of kernel hyperparameters, especially in high dimensions, remains a challenge.

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MS33

A Spatially-correlated Bayesian Gaussian Process Latent Variable Model for Dimensionality Reduction

An increasingly critical ingredient for uncertainty quantification tasks with high-dimensional stochastic spaces is the construction of latent variable models that can discover and represent underlying low-dimensional structure present in the data. Furthermore, one often has knowledge about the stochastic inputs in the form of an implicit model that can be sampled to generate realizations, but does not provide an explicit probability measure over the stochastic space. Such models often provide a picture that is much more realistic than random field models such as Gaussian processes whose appeal lies in ones ability to easily perform dimensionality reduction analytically (e.g. via KLE). In this work, we extend the Bayesian Gaussian process latent variable model [M. Titsias and N. D. Lawrence, AISTATS10] by incorporating explicit prior spatial information into the model reflecting the characteristics commonly found in heterogeneous physical systems while exploiting the spatial structure on which observations are taken to make the method computationally efficient. Our methodology allows us to perform dimensionality reduction with limited data and provides uncertainty estimates about the discovered latent variables thanks to its Bayesian formulation. We demonstrate the utility of the developed model by doing inference on a variety of example data sets and compare its performance to other approaches.

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MS33

Scalable Inference with Transport Maps

Bayesian inference models often result in high-dimensional non-standard distributions, against which there is seldom an efficient and accurate way of computing integrals. We first review the framework of transport maps, where we construct an homeomorphism able to approximate the intractable distribution by a tractable one. Its construction is based on the solution of a variational problem defined over the infinite-dimensional space of monotone transports. We then show how these transports can be used to solve high-dimensional Bayesian inference problems by exploiting their intrinsic low-dimensional structure. Applications in engineering, physics and finance will be used to showcase the methodology.

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MS33

An Approximate Empirical Bayesian Method for Large-scale Linear-gaussian Inverse Problems

Abstract not available at time of publication.

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MS33

A Discrete Sequential Optimal Transport method for Bayesian Inverse Problems

We present the Sequential Ensemble Transform (SET) method for generating approximate samples from a high-dimensional posterior distribution as a solution to Bayesian inverse problems. Solving large-scale inverse problems is critical for some of the most relevant and impactful scientific endeavors of our time. Therefore, constructing novel methods for solving Bayesian inverse problems in more computationally efficient ways can have a profound impact on the science community. This research derives the novel SET method for exploring a posterior by solving a sequence of discrete optimal transport problems, resulting in a series of transport maps which map prior samples to posterior samples, allowing for the computation of moments of the posterior. We show both theoretical and numerical results, indicating this method can offer superior computational efficiency when compared to other Sequential Monte Carlo (SMC) methods. The SET method is shown to be superior to SMC in cases where partical degenercy is more likely to occur.

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MS34

Provably Convergent Multi-fidelity Bayesian Infer-

ence using Adaptive Delayed Acceptance

Abstract not available at time of publication.

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MS34

Incorporating Epistemic Uncertainty from Lower-fidelity Models in Bayesian Inverse Problems

This paper is concerned with the solution of model-based, Bayesian inverse problems. As many other UQ tasks, this is hindered by the significant cost associated with each forward model evaluation and the large number of unknowns. A popular strategy to alleviate these difficulties has been the use of surrogate, lower-fidelity models which are much cheaper to evaluate. Independently of the particulars, the use of such surrogates introduces an additional source of (epistemic) uncertainty. That is, regardless of the amount of training data, the lower-fidelity model is incapable of predicting exactly the output(s) of interest of the reference, high-fidelity model. We adopt an augmented Bayesian strategy that can account for this additional source of uncertainty and reflect it in the posterior of the unknown model parameters. The flexibility in terms of the number and type of lower-fidelity model(s) employed, allows the use of advanced inference strategies making use of derivatives which further alleviate the computational burden. Furthermore, the framework lends itself naturally to adaptive refinements by identifying regions in the unknown parameter space where additional, high-fidelity runs are needed in order to most efficiently refine the estimates obtained. We demonstrate the performance of various Bayesian coupling strategies between low and high-fidelity models in the context of continuum thermodynamics.

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MS34

A Bayesian Interpretation of Kernel-based Methods for Multifidelity Approximation

A recently developed technique for forward uncertainty quantification (UQ) uses the induced reproducing kernel Hilbert space from a low-fidelity parametric model as a tool to understand the parametric variability of a more expensive high-fidelity model. This has been the cornerstone of a multifidelity simulation technique that seeks to attain accuracy comparable to an expensive high-fidelity model with the cost of an inexpensive low-fidelity model. We show that this methodology, explicitly developed for forward UQ problems, has an interesting Bayesian interpretation by introducing suitable notions of prior and posterior distributions.

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MS34

Multifidelity Transport Maps for Bayesian Inference

Computational expense often prevents the use of Bayesian techniques on large time-critical applications. Transport maps, which are nonlinear random variable transformations, can be constructed offline (before collecting data) and thus have the potential to significantly reduce the online (after collecting data) cost of Bayesian inference. The offline construction phase however, can also be computationally intractable. In this work, we outline a new multifidelity approach to sample-based transport map construction. Computational costs and performance are discussed in the context of sea-ice modeling.

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MS35

Mathematical and Statistical Model Misspecifications in Modeling Immune Response in Renal Transplant Recipients

We examine uncertainty in clinical data from a kidney transplant recipient infected with BK virus and investigate mathematical model and statistical model misspecifications in the context of least squares methodology. A difference-based method is directly applied to data to determine the correct statistical model that represents the uncertainty in data. We then carry out an inverse problem with the corresponding iterative weighted least squares technique and use the resulting modified residual plots to detect mathematical model discrepancy. This process is implemented using both clinical and simulated data. Our results demonstrate mathematical model misspecification when both simpler and more complex models are assumed compared to data dynamics.

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MS35

Estimating the Distribution of Random Parameters in, and Deconvolving the Input Signal to, a Diffusion Equation Forward Model for a Transdermal Alcohol Biosensor

The distribution of random parameters in a distributed parameter model with unbounded input and output for the transdermal transport of ethanol is estimated. The model takes the form of a diffusion equation with the input being the blood alcohol concentration (BAC) and the output being the transdermal alcohol concentration (TAC). Our approach is based on the reformulation of the underlying dynamical system in such a way that the random parameters are now treated as additional space variables. When the distribution to be estimated is assumed to be defined in terms of a joint density, estimating the distribution is equivalent to estimating the diffusivity in a multidimensional diffusion equation and thus well-established finite dimensional approximation schemes, functional an-

alytic based convergence arguments, optimization techniques, and computational methods may all be employed. Once the forward population model has been identified or trained based on a sample from the population, the resulting distribution can then be used to deconvolve the BAC input signal from the biosensor observed TAC output signal. In addition, our approach allows for the direct computation of corresponding credible bands without simulation. We use our technique to estimate bivariate normal distributions and deconvolve BAC from TAC based on data from a population that consists of multiple drinking episodes from a single subject and a population consisting of a single episode from multiple subjects.

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MS35

Individual Level Modeling of Uncertainty in Infectious Diseases

Appropriately modeling the uncertainty that underlies individual responses is crucial to building a useful predictive model. Using sparse individual data to scale up and calibrate a population-level model has long been recognized as a challenging and important problem in clinical trials of preventive and therapeutic medicine. Recent efforts have suggested that representing individual data as such, and not as a response from an 'average' individual, provides an improved informative framework, with which to more accurately anticipate successes or failures to proposed intervention strategies.

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MS35

A Review of Algorithmic Tools for Causal Effect Quantification

Researchers in applied statistics have developed a number of methods for the quantification of treatment effect size and variability from observational (i.e., non-experimental) data. However, the these methods suffer two major limitations. First, the proposed models may suffer from misspecifications as a result of marginalizing (unobserved latent confounders) and conditioning (non-random selection effects) relative to the data-generating model. Second, the data collected is often censored or incomplete. As a result of these uncertainties, inference methods associated with such models are inefficient at best and totally incorrect at worst. In this talk, several recent theoretical developments are reviewed with a particular focus on algorithmic considerations for the design of estimators that are both efficient and robust. A few examples will be selected from fields of public health, epidemiology, biology, etc.

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MS36

Gromovs Method for Stochastic Particle Flow Nonlinear Filters

We present a new exact stochastic particle flow filter, using a theorem of Gromov. Our filter is many orders of magnitude faster than standard particle filters for high dimensional problems, and our filter beats the extended Kalman filter accuracy by orders of magnitude for difficult nonlinear problems. Our theory uses particle flow to compute Bayes rule, rather than a pointwise multiply. We do not use resampling of particles or proposal densities or any MCMC method. But rather, we design the particle flow with the solution of a linear first order highly underdetermined PDE. We solve this PDE as an exact formula which is valid for arbitrary smooth nowhere vanishing densities. Gromov proves that there exists a nice solution to a linear constant coefficient PDE for smooth functions if and only if the number of unknowns is sufficiently large (at least the number of linearly independent equations plus the dimension of the state vector). A nice solution of the PDE means that we do not need any integration, and hence it is very fast. To dispel the mystery of Gromovs theorem we show the simplest non-trivial example. We also show several generalizations of Gromovs theorem. Particle flow is similar to optimal transport, but it is much simpler and faster because we avoid solving a variational problem. Optimal transport is deterministic whereas our particle flow is stochastic, like all such algorithms that actually work robustly.

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MS36

A Critical Overview of Controlled Interacting Particle Systems for Nonlinear Filtering

As the first talk in the Minisymposium, I will introduce the control-based feedback particle filter algorithm and describe its relationship to the ensemble Kalman filter (e.g., Reich) as well as other types of particle flow algorithms (e.g., Daum). I will review results from studies that have shown favorable numerical comparisons for the control-based algorithms when compared to the importance sampling based algorithms (e.g., Berntorp, Stano, Surace). I will describe the common aspects of the control-based algorithms, in particular, the partial differential equation (pde) that needs to be solved to obtain the control law. I will carefully describe the associated numerical problem in the interacting particle settings and review the state-of-the-art algorithms for obtaining the solution. I will close with a discussion of open theoretical and numerical problems in this area. Advances on some of these problems (e.g., solution of the pde) will also be discussed as part of the other talks (Meyn, Daum) in the Minisymposium.

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MS36

Feedback Particle Filter and the Poisson Equation

The particle filter is now a standard approximation of the nonlinear filter for discrete time hidden Markov models. The feedback particle filter is a more recent innovation that is also based on particles. The major difference is that the re-sampling step in the standard algorithm is replaced by an innovation gain. This talk will begin with the basic feedback particle filter algorithm, and focus on methods to approximation the gain function K. A fascinating and

valuable representation of the gain is as the gradient of a solution to Poisson's equation. Specifically, under general conditions, $\mathsf{K} = \nabla h$, where h solves

$$\mathcal{D}h = -\tilde{c}\,,$$

$\mathcal{D}$ is the differential generator associated with a Langevin diffusion, and $\tilde{c}$ is the observation function (centered to have zero mean). Poisson's equation arises in many other areas of control and statistics, and there are many approaches available for approximations. Among these is a variant of the celebrated TD-learning algorithm. It is shown that the Langevin generator admits special structure that leads to more efficient approximation techniques based on either a finite dimensional basis or kernel methods.

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MS36

The Neural Particle Filter: Scalability and Biological Implementation

The robust estimation of dynamical hidden features, such as the position of prey, based on sensory inputs is one of the hallmarks of perception. This dynamical estimation can be rigorously formulated by nonlinear Bayesian filtering theory. Recent experimental and behavioral studies have shown that animals performance in many tasks is consistent with such a Bayesian statistical interpretation. However, it is presently unclear how a nonlinear Bayesian filter can be efficiently implemented in a network of neurons that satisfies some minimum constraints of biological plausibility. We argue that the Neural Particle Filter, which is very similar to the Feedback Particle Filter, can serve as a model of filtering by circuits in the brain, and discuss some of the specific problems of interpreting such a particle system as a network of neurons. Special attention is given to the problems of scalability in the number of dimensions and biological plausibility.

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MS37

Optimal Experimental Design using Laplace Based Importance Sampling

In this talk, the focus is on optimizing strategies for the efficient computation of the inner loop of the classical double-loop Monte Carlo for Bayesian optimal experimental design. We propose the use of the Laplace approximation as an effective means of importance sampling, leading to a substantial reduction in computational work. This approach also efficiently mitigates the risk of numerical underflow. Optimal values for the method parameters are derived, where the average computational cost is minimized subject to a desired error tolerance. We demonstrate the computational efficiency of our method, as well as for a more recent approach that approximates using the Laplace method the return value of the inner loop. Finally, we present a set of numerical examples showing the efficiency of our method. The first example is a scalar problem that is linear in the uncertain parameter. The second example is a nonlinear scalar problem. The last example deals with sensor placements in electrical impedance tomography to recover the fiber orientation in laminate composites.

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MS37

Optimal Design of Experiments in the Chemical Industry

Validated dependable mathematical models are of ever growing importance in science and engineering, and today also driven by a serious demand of the industry. In this context the new paradigmatic concept of digital twins may be worth mentioning, which is becoming more and more attractive among researchers from different industrial companies. Its idea is that every new system, product or a physical or economical process should be accompanied by a digital twin, which comprises an ensemble of mathematical models and algorithms. It would ideally accompany the process and be used among others to analyze data, predict malfunctioning and perform optimal operation. However, the application of mathematical models for the simulation, and even more for the optimization and control of complex engineering processes requires their thorough validation and calibration by parameter and state estimation based on process data, which should preferably be obtained by optimized experiments, and optimized measurement designs. For the latter, very efficient numerical methods for the complex non-standard optimal control problem of optimal experimental design for dynamic processes were developed, which have proven to be a powerful mathematical instrument of high economic impact in industrial practice - often cutting experimental costs by a factor of 5 to 10! The talk will especially address numerous applications of model validation methods from chemical engineering.

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MS37

Optimal Experimental Design Problem as Mixed-integer Optimal Control Problem

The optimization of one or more dynamic experiments in order to maximize the accuracy of the results of a parameter estimation subject to cost and other technical inequality constraints leads to very complex non-standard optimal control problems. One of the difficulties is that the objective function is a function of a covariance matrix and therefore already depends on a generalized inverse of the Jacobian of the underlying parameter estimation problem. Another difficulty is that in case of sampling design, we deal with an optimal control problems with mixed-integer controls. We are interested in the application of the Pontryagins maximum principle in order to understand the structure of the sampling design.

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MS37

Generalized Laplace Method for Optimal Experimental Design for Non-Gaussian Posteriors

The Laplace method has been shown to be very efficient in computing the information criteria in the Bayesian design of experiments. The assumption is usually that the posterior distribution concentrates at a single point - the MAP estimate. We extend the Laplace method to two more general scenarios. In the first scenario, the posterior distribution has a compact support thus can be approximated by a truncated Gaussian. In the second scenario, the unknown parameters cannot be fully determined by the data from the proposed experiments, hence the information gain is computed only in the subspace where data is informative.

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MS38

Bayesian Filtering for Periodic, Time-varying Parameter Estimation

Many systems arising in biological applications are subject to periodic forcing. In these systems, the forcing parameter is not only time-varying but also known to have a periodic structure. We show how nonlinear Bayesian filtering techniques can be employed to estimate periodic, time-varying parameters, while naturally providing a measure of uncertainty in the estimation. Results are demonstrated using data from several biological applications.

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MS38

Uncertainty in Estimation using the Prohorov Metric Framework

Glioblastoma Multiforme (GBM) is a malignant brain cancer with a tendency to both migrate and proliferate. We have modeled GBM using a random differential equation version of the reaction-diffusion equation, where the diffusion parameters D and growth rates are random variables. We investigate the ability to perform the inverse problem to recover the probability distributions of D and the growth rates along with measures of their uncertainty using the Prohorov metric. We give a brief overview of use of the Prohorov metric which is equivalent to the weak* topology on the space of probability measures when imbedded in the topological dual of the space of bounded continuous functions. This represents joint efforts with Erica Rutter and Kevin Flores at NCSU.

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MS38

A Bayesian Framework for Strain Identification from Mixed Diagnostic Samples

We present a statistical framework and computational methods for disambiguation of pathogen strains in mixed DNA samples. Our method is relevant for applications in public health and can be used, for example, to identify pathogens and monitor disease outbreak. Mathematically, strain identification aims at simultaneously estimating a binary matrix and a real-valued vector such that their product is approximately equal to the measured data vector. The problem has a similar structure to blind deconvolution, but binary constraints are present in the formulation and enforced in our approach. Following a Bayesian approach, we derive a posterior density and present two MAP estimation methods that exploit the structure of the problem. The first one decouples the problem into smaller independent subproblems, whereas the second one converts the problem to a task of convex mixed-integer quadratic programming. The decoupling approach also provides an efficient way to integrate over the posterior.

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MS38

Physical-model-based, Data-driven Approach Toward Noninvasive Prediction of Intracranial Pressure

Intracranial pressure (ICP) monitoring is clinically significant to patients suffering cerebral decreases. However, clinically accepted ICP measurement data can only be obtained by invasive techniques, which have high risks for patients. Although recent developments in mathematical modeling on the cerebral hemodynamics have enabled us to better understand the mechanisms that drive ICP dynamics, the accuracy of the model predictions is far from being clinically accepted. On the other hand, noninvasive measurement techniques are widely used in clinical practice, and thus more and more ICP-related measurement data become available. In this work, the objective is to leverage the use of both the physical model and ICP-related data to better estimate intracranial dynamics noninvasively. To this end, a simulation-based, data-driven framework is developed based on a multiscale model of cerebral hemodynamics and iterative ensemble Kalman method. Measurement data of cerebral blood flow velocities (CBFV) from noninvasive techniques, e.g., Transcranial Doppler Ultrasound, are assimilated. Numerical results demonstrate the merits of the proposed framework.

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MS39

Data-driven and Reduced Order Modeling : An Attempt at a Taxonomy of Approaches

With the growing interest in data-driven and reduced order approaches, there is a pressing need to classify different problem formulations and approaches using a consistent language. Since this field is inherently multi-disciplinary, even the use of basic terms such as "prediction" or "estimation" tend to be confusing and often misused. In this talk, an attempt is made at establishing a taxonomy of approaches in data-driven and reduced order modeling. Different classes of problems that are addressed by these approaches will be categorized and examples from literature will be provided. The intent of this talk is to set the stage for the use of a common terminology such that the community can - in the future - efficiently navigate literature and more easily exchange ideas.

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MS39

Offline-enhanced Reduced Basis Method through Adaptive Construction of the Surrogate Training Set

The Reduced Basis Method (RBM) is a popular certified model reduction approach for solving parametrized partial differential equations. One critical stage of the offline portion of the algorithm is a greedy algorithm, requiring maximization of an error estimate over parameter space. In practice this maximization is usually performed by replacing the parameter domain continuum with a discrete "training" set. When the dimension of parameter space is large, it is necessary to significantly increase the size of this training set in order to effectively search parameter space. Large training sets diminish the attractiveness of RBM algorithms since this proportionally increases the cost of the offline phase. In this work we propose novel strategies for offline RBM algorithms that mitigate the computational difficulty of maximizing error estimates over a training set. The main idea is to identify a subset of the training set, a "Surrogate Training Set" (STS), on which to perform greedy algorithms. The STS's we construct are much smaller in size than the full training set, yet our examples suggest that they are accurate enough to induce the solution manifold of interest at the current offline RBM iteration. We demonstrate the algorithm through numerical experiments, showing that it is capable of accelerating offline RBM procedures without degrading accuracy, assuming that the solution manifold has rapidly decaying Kolmogorov width.

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MS39

Inverse Regression-based Uncertainty Quantification for High Dimensional Models

Many uncertainty quantification (UQ) approaches suffer from the curse of dimensionality, that is, their computational costs become intractable for problems involving many uncertainty parameters. In these situations, the classic Monte Carlo (MC) often remains the preferred method of choice because its convergence rate $O(n^{1/2})$, where n is the required number of model simulations, does not depend on the dimension of the problem. However, many high-dimensional UQ problems are intrinsically low-dimensional, because the variation of the quantity of interest (QoI) is often caused by only a few latent parameters varying within a low-dimensional subspace, known as the sufficient dimension reduction (SDR) subspace in the statistics literature. Motivated by this observation, we propose two inverse regression-based UQ algorithms (IRUQ) for high-dimensional problems. Both algorithms use an inverse regression method, e.g., the sliced inverse regression (SIR) method, to convert the original high-dimensional problem to a low-dimensional one, which is then efficiently solved by building a response surface for the reduced model, e.g., via the polynomial chaos expansion. While the first algorithm relies on the existence of an exact dimension reduction subspace, the second algorithm applies to a broader set of problems where the dimension reduction is approximate.

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MS39

Dimension Reduction-Accelerated Parameter Estimation

A grand challenge in uncertainty quantification is the solution of inverse problem governing by partial differential equations (PDEs). The forward problem is usually characterized by a large dimensional parameter field. As a result, direct solving this hundred to thousand-parameter problem is computational infeasible. Instead we rely on the Bayesian solution to seek the most probable combination of the parameters. The Markov chain Monte Carlo (MCMC) method provides a powerful tool to generate the posterior distributions of the parameters as well as the most probable point in the parameter space. In this work, we also utilize the gPC surrogates and combine the state to the art dimensional reduction technique to accelerate the MCMC evaluation. The data driven dimensional reduction based on the conditional random field provides a tractable approach to estimate the spatial dependent coefficient with only a few measurements.

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MS40

Efficient Bathymetry Estimation in the Presence of Model and Observation Uncertainties

The high cost and complex logistics of using ship-based surveys for bathymetry estimation have encouraged the use of remote sensing techniques. Data assimilation methods combine the remote sensing data and hydrodynamic models to estimate the unknown bathymetry and the corresponding uncertainties. In particular, several recent efforts have combined Kalman Filter-based techniques such as ensemble-based Kalman filters with indirect video-based observations to address the bathymetry inversion problem. However, these methods often suffer from ensemble collapse and uncertainty underestimation. We present scalable and robust methods for bathymetry estimation problem with the presence of model and observation uncertainty and show the robustness and accuracy of the proposed methods with nearshore bathymetry estimation and river depth imaging examples.

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MS40

Approximate Bayesian Inference under Reduced Model in Inverse Problem and Uncertainty Quantification

Abstract not available at time of publication.

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MS40

Bayesian Inference and Multiscale Model Reduction for Inverse Problems

In the talk, we present a strategy for accelerating posterior inference for statistical inverse problems. In many inference problems, the posterior may be concentrated in a small portion of the entire prior support. It will be much more efficient if we build and simulate a surrogate only over the significant region of the posterior. To this end, we construct a reduced order model, and an intermediate distribution is built using the approximate sampling distribution based on the reduced order model. Then we reconstruct another reduced order based on the intermediate distribution to explore a surrogate posterior. For Bayesian inference, Markov chain Monte Carlo is used to explore the surrogate posterior density, which is based on the surrogate likelihood and the intermediate distribution. The idea is extended to Bayesian data assimilation, where the priors are dynamically updated as more observation date is available. The reduced order model is also dynamically updated in the data assimilation. Compared with the surrogate model directly based on the original prior, the proposed method improves the efficiency of the posterior exploration and reduces uncertainty for parameter estimation and model prediction. The proposed approach is studied in context of multiscale model reduction and applied to the inverse problems for time fractional diffusion models in porous media.

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MS40

An Adaptive Reduced Basis Anova Method for High-dimensional Bayesian Inverse Problems

Abstract not available at time of publication.

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MS41

Ordered Line Integral Methods for Computing the Quasi-potential

The quasi-potential is a key function in the Large Deviation Theory. It characterizes the difficulty of the escape from the neighborhood of an attractor of a stochastic non-gradient dynamical system due to the influence of small white noise. It gives an estimate of the invariant probability distribution in the neighborhood of the attractor up to the exponential order and allows one to readily compute the maximum likelihood escape path. I will present a new family of methods for computing the quasi-potential on a regular mesh in 2D and 3D named the Ordered Line Integral Methods (OLIMs). Similar to Vladimirsky's and Sethian's Ordered Upwind methods, OLIMs employ the dynamical programming principle. Contrary to it, they (i) feature a new hierarchical approach for the use of computationally expensive triangle updates, and (ii) directly solve local minimization problems using quadrature rules instead of solving the corresponding Hamilton-Jacobi-type equation by the first order finite difference upwind scheme.

These differences enable a notable speed-up and a dramatic reduction of error constants (up to 1000 times).

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MS41

Computing the Quasi-Potential in Systems with Anisotropic Diffusion

It is natural to model a number of biological phenomena using SDEs with varying and anisotropic diffusion term. An example is the model for gene regulation in Lambda Phage (Aurell and Sneppel, 2002). The question of interest there is the transition from the phase where the phage reproduces within the cell without killing it to the one where it kills it. I will introduce a modification of an Ordered Line Integral Method for the case of variable anisotropic diffusion for computing the quasi-potential, the key function determining transition rates and Maximum Likelihood Paths (MLPs) in the small noise case. A collection of accuracy tests will be presented. The effects of the anisotropy on the quasi-potential and MLPs will be demonstrated on the Maier-Stein model. Finally, an application of the proposed solver to the analysis of the Lambda Phage gene regulation model will be discussed.

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MS41

Optimal and Robust Control for Piecewise-deterministic Processes.

Piecewise-deterministic (PD) processes provide a convenient framework for modeling non-diffusive stochastic perturbations in a planning environment. (E.g., changes in the wind direction when planning a path for a sailboat.) These stochastic switches are typically modeled through a continuous-time Markov chain on a set of "deterministic modes", with transition probabilities estimated using historical data. This mathematical formalism leads to a system of weakly-coupled PDEs (one for each mode) and additional computational challenges. In this talk we will discuss several notions of optimality and robustness for controlling PD processes, focusing on numerical techniques needed to make them practical. [Joint work with Zhengdi Shen.]

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MS41

Rare Event Study on the Checkpoint Activation in the Budding Yeast Cell Cycle

Abstract not available at time of publication.

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MS42

Compressive Sensing with Cross-validation and Stop-sampling for Sparse Polynomial Chaos Expansions

Compressive sensing is a powerful technique for recovering sparse solutions of underdetermined linear systems, which is often encountered in UQ of expensive and high-dimensional physical models. We perform numerical studies employing several compressive sensing solvers that target the unconstrained LASSO formulation, with a focus on linear systems that arise in the construction of polynomial chaos expansions. With core solvers of l1_ls, SpaRSA, CGIST, FPC_AS, and ADMM, we develop techniques to mitigate overfitting through an automated selection of regularization constant based on cross-validation, and a heuristic strategy to guide the stop-sampling decision. Practical recommendations on parameter settings for these techniques are provided and discussed. The overall method is applied to large eddy simulations of supersonic turbulent jet-in-crossflow involving a 24-dimensional input. Through empirical phase-transition diagrams and convergence plots, we illustrate sparse recovery performance with polynomial chaos bases, accuracy and computational expense tradeoffs between bases of different degrees, and practicability of conducting compressive sensing for a realistic, high-dimensional physical application. We find ADMM to have demonstrated empirical advantages through consistent lower errors and faster computational times.

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MS42

Enhanced Sparse Recovery of Polynomial Chaos Expansions Using Dimension Adaptation and Near-optimal Sampling

Compressive sampling has become a widely used approach to construct polynomial chaos surrogates when the number of available simulation samples is limited. Originally, these expensive simulation samples would be obtained at random locations in the parameter space. In this presentation, we discuss algorithms that can be used to (1) reduce the dimensionality of the polynomial representation and (2) identify the sample locations in a proper way. The proposed dimension reduction approach incrementally explores subdimensional expansions for a sparser/more accurate recovery. The near-optimal algorithm builds upon coherence-optimal sampling, and identifies near-optimal sample locations that lead to enhancement of cross-correlation properties of the measurement matrix. We provide several numerical examples to demonstrate the proposed strategies produce substantially more accurate results, compared to other strategies in the literature.

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MS42

Time and Frequency Domain Methods for Sparse Basis Selections in Random Linear Dynamical Systems

We consider linear dynamical systems consisting of ordinary differential equations with random variables. A quantity of interest is defined as an output of the system. We represent the quantity of interest in a polynomial chaos expansion, which includes orthogonal basis polynomials. Now the aim is to determine a low-dimensional approximation (or sparse approximation), where just a few basis polynomials are required for a sufficiently accurate representation of the quantity of interest. We investigate a time domain method and a frequency domain method for the identification of a low-dimensional approximation. On the one hand, the stochastic Galerkin method is applied to the random linear dynamical system. A frequency domain analysis of the Galerkin system yields a measure for the importance of basis polynomials and thus a strategy for the selection of basis functions. On the other hand, a sparse minimization chooses the basis polynomials by information from the time domain only. Therein, an orthogonal matching pursuit produces an approximate solution of the minimization problem. The two approaches are compared using a test example from a mechanical application. Numerical results are presented. In particular, we illustrate the choice of the basis polynomials in the two methods.

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MS42

High-dimensional Function Approximation Via Weighted L1 Minimization with Gradient-augmented Samples

Many physical problems involve approximating high-dimensional functions with a limited number of sampling points. It is seen that the high-dimensional function interpolation problem has various applications such as uncertainty quantification. For example, in order to compute a quantity of interest for the parametric PDE, high-dimensional function approximation is often required. In this talk, we present the work of interpolating a high-dimensional function using the weighted ℓ^1 minimization technique when both points for the original function and its derivatives are sampled. With additional derivative information, we see a numerical improvement over the case only samples points from the original function. Theoretically, we show that with exactly the same complexity as in the case of function samples only, the gradient enhanced method gives a better error bound in the Sobolev-type norm as opposed to the $L2$ norm.

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MS43

Multi-reduction MCMC Methods for Bayesian Inverse Problem

We propose a Monte-Carlo methods for Bayesian inverse problem with nested reduced-order models. Details assumptions and rigorous proofs on the efficiency of the proposed multi-reduction MCMC will be provided. Numerical results will be presented to validate the theoretical approaches.

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MS43

Multilevel DILI

In this paper we combine two state-of-the-art MCMC algorithms: Multilevel MCMC (MLMCMC) and Dimension-Independent Likelihood-Informed (DILI) MCMC. Both these algorithms have been shown to significantly improve on existing MCMC algorithms in the context of high-dimensional PDE-constrained Bayesian inverse problems. We will show that the gains of the two approaches are complementary and that the combination of the two outperforms each of the individual algorithms. While MLMCMC reduces the computational cost by shifting most of the work from high-fidelity approximations of the underlying PDE to coarser and cheaper ones, DILI uses low-rank approximations of the Hessian of the posterior to obtain good proposals within the core MCMC step. In particular, in DILI MCMC the high-dimensional parameter space is split into a low-dimensional Likelihood-Informed Subspace and its complement, resulting in low rejection rates and fast mixing. We show that a hierarchy of likelihood-informed subspaces across the different levels of the MLMCMC algorithm can be defined consistently and updated cheaply, even when the number of parameters increases as the level increases. We introduce a proposal scheme that asymptotically converges to the correct posterior distribution of the parameters on each level, given the distribution of the parameters on the coarser levels, even when the input random field is not parametrised via a Karhunen-Loève expansion. Numerical experiments confirm the gains.

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MS43

Multilevel Ensemble Transform Methods for

Bayesian Inference

Ensemble transform methods are useful frameworks for a Bayesian approach to data-assimilation. For example, an Ensemble Transform Particle Filter (ETPF) uses a deterministic transform from forecast to analysis ensembles at each assimilation step, instead of a traditional random resampling step. With the use of localisation, one can also extend the scheme to high-dimensional cases. This provides a framework to implement data-assimilation on PDEs containing random coefficients or that have trajectories modelled by a Brownian Motion. However the computational cost of propagating ensembles of realisations of these PDEs can be very large. This talk details algorithms to apply the efficient multilevel Monte Carlo (MLMC) approach to ensemble transform methods, in particular the ETPF; discussing its effectiveness. The challenge here is being able to couple the analysis ensembles of the coarse and fine discretizations in the MLMC framework; this is an active area of research. Through proof of concepts, the algorithms considered are shown to speed-up the propagation of ensembles within filtering estimators, with a fixed order of accuracy, from their standard counterparts.

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MS43

Multilevel Sequential^2 Monte Carlo for Bayesian Inverse Problems

The identification of parameters in mathematical models using noisy observations is a common task in uncertainty quantification. We employ the framework of Bayesian inversion: we combine monitoring and observational data with prior information to estimate the posterior measure of a parameter. Specifically, we are interested in the probability measure of a diffusion coefficient of an elliptic partial differential equation. In this setting, the sample space is high-dimensional, and each sample of the solution of the partial differential equation is expensive. To address these issues we propose a novel Sequential Monte Carlo sampler for the approximation of the posterior measure. Classical, single-level Sequential Monte Carlo constructs a sequence of probability measures, starting with the prior measure, and finishing with the posterior measure. The intermediate probability measures arise from a tempering of the likelihood, or, equivalently, a rescaling of the noise. The resolution of the discretisation of the partial differential equation is fixed. In contrast, our estimator employs a hierarchy of discretisations to decrease the computational cost. Importantly, we construct a sequence of intermediate probability measures by decreasing the temperature and increasing the discretisation level at the same time. We present numerical experiments in 2D space and compare our estimator to single-level Sequential Monte Carlo and other alternatives.

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MS44

Improving Sub-grid-scale Approximations in Global Atmospheric Models using Data-driven Techniques

Direct numerical simulation of the atmosphere and ocean on any spatial or temporal scale of interest is not feasible given the inherently turbulent nature of the dynamics. Because a typical climate model has a horizontal grid size of 160km, which is far larger than the turbulent dissipation scale, it uses approximate closures to represent unresolved dynamics. In particular, moist atmospheric convection is amongst the most important unresolved processes, but its multiscale behavior severely challenges traditional approaches based on simplified physical modeling. To circumvent these issues, we have developed a regression based approach to convective closure using a near-global atmospheric simulation with a cloud-permitting resolution (4km) as a training dataset. The large size of the domain allows a two-way coupling between convection and the large-scale circulation. First, we coarse-grain the model variables into 160 km grid boxes. Then, we diagnose a simple linear model which regresses the coarse-grained source terms onto the average vertical profiles of humidity, temperature, and velocity in each horizontal grid cell. This model is able to explain about 40% of the observed variance of the source terms, and we further test its performance by using it as the closure in a prognostic coarse-resolution simulation.

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MS44

Data-driven Determination of Koopman Eigenfunctions using Delay Coordinates

The Koopman operator induced by a dynamical system provides an alternate method of studying the system as an infinite dimensional linear system, and has applications to attractor reconstruction and forecasting. Koopman eigenfunctions represent the non-mixing component of the dynamics. They factor the dynamics, which can be chaotic, into quasiperiodic rotation on tori. Here, we describe a method in which these eigenfunctions can be obtained from a kernel integral operator, which also annihilates the continuous spectrum. We show that incorporating a large number of delay coordinates in constructing the kernel of that operator results, in the limit of infinitely many delays, in the creation of a map into the discrete spectrum subspace of the Koopman operator. This enables efficient approximation of Koopman eigenfunctions from high-dimensional data in systems with point or mixed spectra.

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MS44

Parsimonious Model Selection using Genomic Data for Outbreak Intervention

We discuss novel computational methods for tracking disease in human populations using pathogen genomes. Population models of disease are often studied as complex dynamical systems with many nonlinear interactions. A full mechanistic modeling perspective would incorporate all scales of the system from intra-host pathogen behavior to inter-host social network structure. We have instead concentrated on parsimonious models complemented by fast algorithms that can potentially enable meaningful intervention decisions. We built a likelihood-based nested model selection framework for virus mobility informed by linked pathogen genome sequences. Then we demonstrated our methodology on Ebola virus genomes collected from Sierra Leone during the 2013-2016 outbreak in West Africa. We discovered that the outbreak showed a temporal change in model preference coincident with a documented intervention, the Western Area Surge.

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MS44

Improving Accuracy and Robustness of Artificial Neural Networks to Discover Dynamical Systems from Data

Despite the successful application of machine learning (ML) in fields such as image processing and speech recognition, only a few attempts has been made toward employing ML to discover/represent the dynamics of complex physical systems. In this work, we study the use of artificial neural networks to a) discover dynamical systems from data, and b) to discover sub-scale dynamics in reduced order models of dynamical systems and point out several critical issues with existing ML techniques. We propose novel approaches to improve predictive capabilities and robustness of neural networks for applications in non-linear dynamical systems. The use of cascading cost functions and global regularization will be discussed in detail.

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MS45

Sensitivity Analysis for Flocking and Synchronization Models

In this talk, we first introduce two random flocking and synchronization models, namely random Cucker-Smale model and random Kuramoto model and then present local sensitivity analysis for those models based on the uniform stability analysis and propagation of Sobolev regularity in random parameter space. This is a joint work with Shi Jin (UW-Madison) and Jinwook Jung (SNU).

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MS45

Hypocoercivity Based Sensitivity Analysis and Spectral Convergence of the Stochastic Galerkin Approximation to Collisional Kinetic Equations with Multiple Scales and Random Inputs

In this talk, the speaker will present a general framework to study a general class of linear and nonlinear kinetic equations with random uncertainties from the initial data or collision kernels, and their stochastic Galerkin approximations, in both incompressible Navier-Stokes and Euler (acoustic) regimes. First, we show that the general framework put forth in [C. Mouhot and L. Neumann, *Nonlinearity*, 19, 969-998, 2006; M. Briant, *J. Diff. Eqn.*, 259, 6072-6141, 2005] based on hypocoercivity for the deterministic kinetic equations can be adopted for sensitivity analysis for random kinetic equations, which gives rise to exponential convergence of the random solution toward the (deterministic) global equilibrium. Then we use such theory to study the stochastic Galerkin (SG) methods for the equations, establish hypocoercivity of the SG system and regularity of its solution, and spectral accuracy and exponential decay of the numerical error of the method in a weighted Sobolev norm. This is a joint work with Shi Jin.

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MS45

Bayesian Estimation for Transport Equations for Nanocapacitors

We use and evaluate different Bayesian estimation methods to quantify uncertainties in model parameters in nanocapacitors. Here, randomness arises due to process variations; also, parameters that cannot be measured directly are to be determined.
The methods include the direct approach, the Markov-chain Monte-Carlo (MCMC) method, and an iterative version of the latter that we have developed, where we use the calculated posterior distribution as the prior distribution for a new MCMC analysis. We investigate the influence of the number of samples in each Markov chain and the number of iterations on the total computational work and the error achieved. In addition, we discuss the methods for estimating the posterior distribution based on samples provided by the MCMC analysis.
We apply our algorithms to the Poisson-Boltzmann and Poisson-Nernst-Planck equations which arise from modeling nanoelectrode biosensors, which have recently been used to detect minute concentrations of target particles. This technology has many applications in precision medicine. Numerical examples show the estimation of parameters such as ionic concentration, size of Stern layer, and the sizes of multiple electrodes (multilevel Bayesian estimation) of sensors for which experimental data are available.

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MS46

Weighted Reduced Order Methods for Parametrized PDEs with Random Inputs

In this talk we discuss a weighted approach for the reduction of parametrized partial differential equations with random input, focusing in particular on weighted approaches based on reduced basis (wRB) [Chen et al., SIAM Journal on Numerical Analysis (2013); D. Torlo et al., submitted (2017)] and proper orthogonal decomposition (wPOD) [L. Venturi et al., submitted (2017)]. We will first present the wPOD approach. A first topic of discussion is related to the choice of samples and respective weights according to a quadrature formula. Moreover, to reduce the computational effort in the offline stage of wPOD, we will employ Smolyak quadrature rules. We will then introduce the wRB method for advection diffusion problems with dominant convection with random input parameters. The issue of the stabilization of the resulting reduced order model will be discussed in detail.

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MS46

Optimal Approximation of Spectral Risk Measures with Application to PDE-constrained Optimization

Many science and engineering applications require the control or design of a physical system governed by partial differential equations (PDEs). More often then not, PDE inputs such as coefficients, boundary and initial conditions, and modeling assumptions are unknown, unverifiable or estimated from data. Such problems can be formulated as risk-averse optimization problems in Banach space. In this talk, I concentrate on spectral risk measures for PDE-constrained optimization. In particular, I develop an optimal quadrature approximation of spectral risk measures. This approximation is provably convergent and results in a consistent approximation of the original optimization problem. In addition, I show that a large class of spectral risk measures can be generated through the risk quadrangle. I conclude with numerical examples confirming these results.

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MS46

Two Basic Hierarchical Structures Making Stochastic Programming What It Is

Two fundamentally different lines of recurring structures in stochastic programming are reported. Behind the first there is the idea of recourse, from its simplest occurrence, consequently called the same way, to settings considered advanced structures either due to the decision pattern (two-stage, multi-stage) or the complexity of the decision spaces. The second line comes from discrete mathematics and occurs when recourse involves combinatorial decisions. In different levels of abstraction, it is the fact that below any positive integer there are at most finitely many others. Under the names of Dickson and Gordan the principle/lemma is forming a cornerstone of symbolic computation.

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MS46

Estimation of Tail Distributions Using Quantile and Superquantile (CVaR) Values

We minimized superquntile (CVaR) of a system described by PDEs with uncertain parameters. Quantile and superquantile (CVaR) were estimated with a small number of samples (e.g. 20 samples). The paper discusses approaches for estimating and minimizing low probability characteristics, such as quantile and superquantile (CVaR) with high confidence levels (e.g., 0.999).

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MS47

Reduced-order Stochastic Modeling and Non-Gaussian Data Assimilation for Marine Ecosystems

Characterizing and predicting ocean phenomena that are high-dimensional and have significant uncertainties, such as marine ecosystems, requires computationally efficient models. We utilize an efficient method for simultaneous estimation of state variables, parameters, and model equations for a regional ocean model coupled with a biogeochemical model. The method uses a generalization of the Polynomial Chaos and Proper Orthogonal Decomposition equations, the dynamically orthogonal (DO) evolution equations, for probabilistic predictions, and a Gaussian mixture model DO (GMM-DO) filtering algorithm for Bayesian data assimilation and inference. We showcase results for Southern New England and the Mid-Atlantic Bight using a regional modeling system that predicts marine ecosystem dynamics using primitive equations coupled to a biogeochemical model. We then discuss the results of the joint estimation of the system's state variables and

parameter values, with learning of the form of the biogeochemical equations. Advisor: Pierre Lermusiaux and Abhinav Gupta, Massachusetts Institute of Technology, USA

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MS47

Statistical Modelling of Breast Cancer Risk for Greater Predictive Accuracy

With 1 in 8 women in the United States at risk of being diagnosed with breast cancer at some point in her lifetime, the development and accuracy of breast cancer prediction models is pertinent to reducing the morbidity and mortality rates associated with the disease. Three such prediction models are the Gail, BCSC (Breast Cancer Surveillance Consortium), and Tyrer-Cuzick models, each of which determine a woman's risk of breast cancer from risk factors including family history of cancer and mammographic density. However, these models have been shown to vary in accuracy among women with different ethnic backgrounds, which is why the Athena Breast Health Network, an extensive program at UCI that integrates clinical care and research to drive innovation in the prevention of breast cancer, is building and testing new breast cancer risk assessment models using machine learning. Experimenting with algorithms such as k-nearest neighbors (KNN), support vector machines (SVM), and decision trees (DT), Athena hopes to evaluate new breast cancer risk models and their predictive accuracies. Advisor: Argyrios Ziogas and Hanna Lui Park, University of California, Irvine, USA

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MS47

Subsurface Impedance Characterization with Bayesian Inference

Methods for directly observing the evolution of a snowpack and the movement of water through snow are required for validating remote sensing and modeling estimates. The density and water content of snow are closely related to its electrical properties, thus Electrical Impedance Tomography (EIT) can be used to characterize the subsurface properties. In this work, a computational feasibility study was conducted to determine if a sensing instrument utilizing EIT can be used to learn about the electrical properties of its surroundings. We apply statistical methods, such as Bayesian inference, to this inverse problem by characterizing the uncertainty that remains in the electrical properties after taking into account voltage observations from the instrument. Advisor: Matthew Parno, US Army Cold Regions Research and Engineering Laboratory (CRREL)

Cassie Lumbrazo
Clarkson University
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MS47

Dynamic Sequential Filtering in Association with Joint State-parameter Estimation

We are proposing a surrogate based strategy for joint state-parameter estimation via sequential filtering. Our approach starts with an ensemble Kalman filter estimate of the prior density. Typically one then applies the Kalman update incorporating the next observation to obtain a posterior estimate. Instead we will incorporate a surrogate model at this stage which will enable a through sampling of the prior and allow for a particle filter type update of the posterior. We will apply this strategy to Lorenz-96 model as proof-of-concept. Mentor: Dr. Elaine Spiller, Marquette University, USA

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MS47

Eulerian vs Lagrangian Data Assimilation

Data assimilation is a process by which a physical model and observational data are combined to produce a more accurate estimate of the state of a system. It is often used when uncertainty (e.g., noise) is present in the systems evolution or in the observational data. For these types of systems, numerical methods must quantify this uncertainty in addition to estimating the mean behavior of the system. Examples of the successful application of data assimilation include predicting weather patterns and ocean currents. We apply a specific data assimilation technique, the Discrete Kalman Filter, to estimate a velocity field. We demonstrate how blending a model with data allows us to infer the state of the system with better accuracy than either the model or the data alone would provide. We simulate the estimation of flow fields with different types of observers (floating versus fixed in space) and observational data (position versus velocity measurements) to analyze the effects this has on estimation skill. Advisor: Richard Moore

MS48

Goal Oriented Sensitivity Indices and Sensitivity Indices Based on Wasserstein Costs

Abstract not available at time of publication.

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MS48

Sensitivity Analysis Based on Cramr Von Mises Distance

In this talk, following an idea of Borgonovo and co-authors in 2007, we define and study a new sensitivity index based on the Cramr von Mises distance. This index appears to be more general than the Sobol one as it takes into account the whole distribution of the random variable and not only the variance. Furthermore, we study the statistical properties of its Pick and Freeze estimator.

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MS48

Statistical Methodology for Second Level Sensitivity Analysis with Dependence Measures for Numerical Simulators

Many physical phenomena are modeled by numerical simulators, which take several uncertain parameters as inputs and can be time expensive. Global sensitivity analyses are then performed to evaluate how the input uncertainties contribute to the variation of the code output. For this, we focus here on dependence measures based on reproducing kernel Hilbert spaces (HSIC). In some cases, the distributions of the inputs may be themselves uncertain and it is important to quantify the impact of this uncertainty on global sensitivity analysis results. We call it the second-level sensitivity analysis. To achieve this, we propose a statistical methodology based on a single Monte Carlo loop: First, we draw a unique sample S built from a unique (suitably chosen as a reference) probability distribution of the inputs and the computation of corresponding code outputs. Then, for various probability distributions of the input parameters, we perform a global sensitivity analysis: HSIC are computed from sample S and using modified estimators. Finally, we realize the 2nd-level sensitivity analysis by estimating 2nd-level HSIC between the probability distributions of the inputs and the results of global sensitivity analysis. For this, specific kernels are chosen. We apply this methodology on an analytical example to evaluate the performances of our procedures and illustrate how it allows for an efficient 2nd-level sensitivity analysis with very few computer experiments.

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MS48

Sensitivity Indices for Outputs on a Riemannian Manifold

Abstract not available at time of publication.

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MS49

Ensemble Filtering with One-step-ahead Smoothing

Ensemble Kalman filters (EnKFs)sequentially assimilate data into a dynamical model to determine estimates of its state and parameters. At each EnKF assimilation cycle, an ensemble of statesis first integrated forward with the model for forecasting. The forecasted ensemble is thenupdated with incoming observations based on a Kalman correction step. The forecast-update cycle is however not the onlypathway to compute the state analysis. Here we reverse the order of these steps followingthe one-step-ahead (OSA) smoothing formulation of the Bayesian filtering problem to propose a new class of EnKFs that constrain the state-parameters ensembles with futureobservation. Exploiting future observations should bring in more information that help mitigating for the suboptimal character of the EnKFs; being formulated for linear and Gaussian systems, and implemented with limitedensembles and crude approximate noise statistics. We further extend the OSA-EnKF framework to biasestimation and for efficient assimilation into one-way coupled models. Numerical results of various applicationswill be presented to demonstrate the efficiency of theof the proposed approach.

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MS49

Non-Gaussian Data Assimilation through Kernel Density Estimation

Non-Gaussian features are typical in many application areas of data assimilation such as geophysical fluid systems and thus it is essential to effectively capture the Non-Gaussian features for accurate and stable state estimates. We compare particle filters and ensemble-based methods and propose a new class of data assimilation using Kernel density estimation that can captures non-Gaussian features effectively using relatively a small number of samples and is robust and stable for high-dimensional problems.

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MS49

Localization for MCMC Sampling High-dimensional Posterior Distributions with Banded Structure

We investigate how ideas from covariance localization in numerical weather prediction can be used to efficiently sample high-dimensional distributions with banded covariance and precision matrices. The main idea is to exploit banded structure during problem formulation and Markov chain Monte Carlo (MCMC) sampling. In particular, we propose to solve high-dimensional Bayesian inverse problems with nearly banded structure (i.e., small off-diagonal

elements) by first replacing the problem with a banded version, setting small off-diagonal elements to zero, and then solving the modified problem using a Metropolis-within-Gibbs sampler that exploits this banded structure. We discuss conditions under which posterior moments of the modified problem are close to those of the original problem. Under the same conditions, the convergence rate of an associated sampler is independent of dimension. We present our ideas in the context of Gaussian problems, where mathematical formulations are precise and for which convergence analysis can be made rigorous.

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MS49

Model Parameter Estimation using Nonlinear Ensemble Algorithms

It is now generally acknowledged that introducing variability in parameters in an ensemble data assimilation and prediction context can increase the realism of the prediction system. However, parameter perturbation is complicated. Many parameters are nonlinearly related to the model output, transfer functions that map from state to observation space may also be nonlinear, and prior parameter distributions may be poorly known and are often bounded at zero. Our approach to parameter estimation uses a Markov chain Monte Carlo (MCMC) algorithm to sample the Bayesian posterior distribution of model parameters. We then test approximate data assimilation methodologies that are less computationally expensive using the MCMC posterior distribution as a reference. In this presentation, we show results from parameter estimation experiments using a MCMC algorithm. We demonstrate the various types of nonlinearity present in cloud microphysical parameterizations, in particular. We then show results from various ensemble filter algorithms, including the Ensemble Transform Kalman Filter (ETKF), and a newly developed filter based on Gamma and Inverse Gamma distributions (the Gamma - Inverse Gamma (GIG) filter). The ETKF exhibits well known problems associated with nonlinearity in the parameter - model state relationship. In contrast, the GIG produces a posterior estimate that is more accurate in both state and observation space, and closely approximates the Bayesian solution generated by MCMC.

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MS50

Hierarchical Bayesian Sparsity: ℓ_2 Magic.

Hierarchical Bayesian models with suitable choices of hyperpriors, combined with Krylov subspace iterative solvers can be very effective at promoting sparsity in the solution of inverse problems while retaining the ℓ_2 computational efficiency. In this talk we will present some results about the convergence of these methods for different families of hyperpriors and show related computed examples.

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MS50

Large Scale Spatial Statistics with SPDEs, GMRFs, and Multi-scale Component Models

Combining multiple and large data sources of historical temperatures into unified spatio-temporal analyses is challenging from both modelling and computational points of view. This is not only due to the size of the problem, but also due to the highly heterogeneous data coverage and the latent heterogeneous physical processes. The EUSTACE project will give publicly available daily estimates of surface air temperature since 1850 across the globe for the first time by combining surface and satellite data using novel statistical techniques. Of particular importance is to obtain realistic uncertainty estimates, due to both observation uncertainty and lack of spatio-temporal coverage. To this end, a spatio-temporal multiscale statistical Gaussian random field model is constructed, with a hierarchy of spatially non-stationary spatio-temporal dependence structures, ranging from weather on a daily timescale to climate on a multidecadal timescale. Connections between SPDEs and Markov random fields are used to obtain sparse matrices for the practical computations. The extreme size of the problem necessitates the use of iterative solvers, which requires using the multiscale structure of the model to design an effective preconditioner. We will also discuss some new computational developments towards full Bayesian estimation of the dependence parameters, and fast computation of posterior predictive variances.

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MS50

Hierarchical Stochastic Partial Differential Equations for Bayesian Inverse Problems

We construct hierarchical models based on stochastic parameters and Gaussian Markov random fields (GMRF). By stacking two GMRFs via their stochastic partial differential equation presentation, we can make the hierachical model suitable for large-scale problems. We choose the prior field to be Matrn, and we study hyperprior field models for the Matrn prior length-scale field. One choice, for a one-dimensional problem, is exponentially distributed hyperprior process, and we give it as autoregressive AR(1) process to keep the computational complexity to minimal. We treat measurement noise variance and hyperprior parameters as unknowns in the posterior distribution. Hyperparameters and hyperpriors tend to be strongly coupled a posteriori, which leaves vanilla MCMC algorithms inefficient. Hence, we propose two MCMC algorithms for the different hierarchical models, which are both free of parameter tuning. One, corresponds to an adaptive Metropolis-within-Gibbs scheme, and the other one employs Elliptical Slice Sampling combined with a reparametrisation to decouple hyperparameters. The developed methodology permits computationally efficient inference and uncertainty quantification about all the estimates in the model. We apply methodology developed to interpolation and X-ray tomography.

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MS50

Hierarchical Gaussian Processes in Bayesian Inverse Problem

A major challenge in the application of sampling methods in Bayesian inverse problems is the typically large computational cost associated with solving the forward problem. To overcome this issue, we consider using a Gaussian process emulator to approximate the forward map. This results in an approximation to the solution of the Bayesian inverse problem, and more precisely in an approximate posterior distribution. In this talk, we analyse the error in the approximate posterior distribution, in the case where the hyper-parameters specifying the Gaussian process emulator are unknown and learnt on the fly from evaluations of the forward model.

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MS51

Goal-oriented Optimal Design of Experiments for Bayesian Inverse Problems

Computer models play an essential role in forecasting complicated phenomena such as the atmosphere, ocean dynamics, volcanic eruptions among others. These models however are usually imperfect due to various sources of uncertainty. Measurements are snapshots of reality that are collected as an additional source of information. Parameter inversion and data assimilation are means to fusing information obtained from measurement, model, prior knowledge, and other available sources to produce reliable and accurate description (the analysis) of the underlying physical system. The accuracy of the analysis is greatly influenced by the quality of the observational grid design used to collect measurements. Sensor placement can be viewed as optimal experimental design (OED) problem, where the locations of the sensors define an experimental design. There are many criteria for choosing an optimal experimental design, such as minimization of the uncertainty in the output (e.g., minimization of the trace of the posterior covariance). Including the end-goal (predictions) in the experimental design leads to a goal-oriented OED approach that can be used in several applications. In this talk, we outline the idea of goal-oriented optimal design of experiments for PDE-based Bayesian linear inverse problems. We also present numerical results from a standard advection-diffusion problem.

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MS51

Bayesian Experimental Design for Stochastic Biochemical Systems

Getting deep and meaningful insights into the function of biological systems requires careful experimental setups. While technological advances have frequently led to fishing expeditions the complexity of e.g. a cell or tissue mean that such data often lacks the power to elucidate underlying mechanisms. In this context simulation-based experimental design is increasingly being recognized as a promising route for detailed analyses of cellular behaviour. In silico simulations are then used, for example, to design experiments that allow us to estimate the parameters of mathematical models describing biophysical and biochemical systems. So far, however, most of these approaches have focused on deterministic modelling approaches. Here we discuss a generalization that addresses the particular problems faced when dealing with stochastic dynamical systems. An information theoretical framework is used to identify experimental conditions that maximise the mutual information between experimental data, and the parameters describing the stochastic dynamical system. We illustrate our approach on a set of exemplar models of stochastic molecular systems.

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MS51

Optimal Experimental Design for RKHS Based Correction of Mis-specified Dynamic Models

All models are wrong, yet, our goal in this study is to infer a functional correction for a mis-specified dynamic model, where the systems dynamics is only known approximately. Here two questions can be considered: what would be an effective functional form to represent the correction term? And given such, how the corrected model can be learnt efficiently, given a limited experimental budget? Assuming the availability of observations of the system for various initial conditions, we propose a formulation for estimating correction terms in a Reproducing Kernel Hilbert Space

(RKHS) of candidate correction functions. Further, we analyze the problem of performing efficient experimental design to find an optimal correction term under a limited experimental budget and experimental constraints. The problem is computationally intractable when formulated in the D-Bayes optimality framework. However, by introducing a suitable approximate proxy, the problem can be cast as a sub-modular optimization problem, for which there are computationally efficient and approximately optimal solvers. Numerical experiments exemplify the efficiency of these techniques.

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MS51

Subspace-driven Observation Selection Strategies for Linear Bayesian Inverse Problems

Many inverse problems may involve a large number of observations. Yet these observations are seldom equally informative; moreover, practical constraints on storage, communication, and computational costs may limit the number of observations that one wishes to employ. We introduce strategies for selecting subsets of the data that yield accurate approximations of the inverse solution. This goal can also be understood in terms of optimal experimental design. Our strategies exploit the structure of inverse problems in the Bayesian statistical setting, and are based on optimal low-rank approximations to the posterior distribution—extended to the observation space.

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MS52

Filtering Without a Model and Without an Observation Function: Data-driven Filtering

Modern methods of data assimilation rely on two key assumptions: that a mathematical model of the physical system and an observation function (which maps the model state to the measurements) are both known. In absence of either, outright implementation of standard techniques such as ensemble Kalman filtering is impossible or subject to large error. In this talk, we will present recent advances in data-driven filtering which attempt to solve these extreme problems in data assimilation.

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MS52

Sensitivity of Network Dynamics Reconstruction

Consider a dynamical network that is observed at a subset of network nodes. If the network is strongly connected, the dynamics at all unobserved nodes can generically be reconstructed, in theory. However, the conditioning of the reconstruction will vary depending on the relation of the observed to unobserved nodes, and reconstruction at some nodes may be difficult in practice. A variational data assimilation method is used to quantify this conditioning based on the observation subset, and the effect of network geometry is discussed.

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MS52

Nonlinear Kalman Filtering for Parameter Estimation with Censored Observations

The use of Kalman filtering, as well as its nonlinear extensions, for the estimation of state variables and model parameters has played a pivotal role in many fields of scientific inquiry where observations of the system are restricted to a subset of variables. However in the case of censored observations, where measurements of the system beyond a certain detection point are impossible, the estimation problem is complicated. Without appropriate consideration, censored observations can lead to inaccurate estimates. In this talk, we present a modified version of the extended Kalman filter to handle the case of censored observations in nonlinear systems. We validate this methodology in a simple oscillator system first, showing its ability to accurately reconstruct state variables and track system parameters when observations are censored. Finally, we utilize the nonlinear censored filter to analyze censored datasets from patients with hepatitis C and human immunodeficiency virus.

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MS52

Parameter Estimation using Linear Response Statistics - Theory and Numerical Scheme

We propose a new parameter estimation method for Itô diffusions using linear response statistics. In this talk, the theory will be briefly reviewed, and a corresponding practical numerical scheme based on the idea of surrogate model will be introduced together with some sensitivity analysis. As an important example, the Langevin system will be discussed in depth.

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MS53

A Data Driven Approach for Uncertainty Quantification with High Dimensional Arbitrary Random Data

One of the grand challenges in uncertainty quantification roots in the implicit knowledge of underlying distribution function of the complex system. Traditional approaches show limitations to quantify the uncertainty propagation associated with such systems. We develop a data-driven approach to accurately construct the surrogate model for the quantify of interest, which is irrespective of the dependency and the analytical form of the underlying distribution. Our method is demonstrated in challenging problem such high-dimensional PDE systems and realistic biomolecule system, and can be generalized to other systems with high dimensional arbitrary random space.

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MS53

Multi-fidelity Uncertainty Propagation of Physics-based Nondestructive Measurement Simulations using Co-kriging

Probability of detection (POD) is a widely established method for measuring the reliability of nondestructive evaluation (NDE) systems. Typically, POD is determined experimentally. However, POD methods can be enhanced by utilizing information from physics-based computational measurement simulations. These are called model-assisted POD (MAPOD) methods. The main elements of MAPOD methods are (1) identify a set of uncertainty input parameters and their probability distributions, (2) propagate the uncertain parameters through the computational models, and (3) build POD curves. One of the key challenges of performing MAPOD with accurate physics-based measurement simulations is the computational expense. In particular, the computational models are time-consuming to evaluate and the process of propagating the uncertain input parameters, Step 2 in the MAPOD process, needs a large number of evaluations using conventional approaches. This talk presents the use of multi-fidelity modeling to accelerate the uncertainty propagation process of the MAPOD analysis. In particular, co-kriging is utilized to fuse information from models of varying degree of fidelity to construct a fast surrogate model, which is utilized for the uncertainty propagation with Monte Carlo sampling (MCS). The approach is demonstrated on MAPOD analysis problems using ultrasonic testing simulations and eddy current simulations. The proposed approach is compared with direct MCS, and MCS with Kriging surrogate models.

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MS53

Bi-directional Coupling between a PDE-domain and an Adjacent Data-domain Equipped with Multi-fidelity Sensors

The increasing collection of data in essentially all facets of our lives has heralded concomitant growth in statistical and machine learning (ML) techniques to analyze the data. Researchers are looking for data-driven algorithms that will solve a partial differential equation (PDE) as an inverse problem. However, few focuses on combining the information provided by the traditional PDE solver and the big data. In this work we are devoted to propagating information between those two paradigms, and specifically, we address on coupling the solution of a PDE governed domain with the big data domain. Our method builds upon the Schwarz alternating method and the recent work on numerical Gaussian process regression (GPR). We further extend our method to deal with data with variate fidelities, using an auto-regressive multi-fidelity model. The effectiveness of our domain decomposition algorithm is demonstrated using examples of Helmholtz equations in both 1D and 2D domains.

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MS54

Exploiting Ridge Approximations for Bayesian Inference

Inexpensive surrogates are key for reducing the cost of parameter studies involving large-scale, complex computational models with many input parameters. A ridge approximation is one class of surrogate that models a quantity of interest as a nonlinear function of a few linear combinations of the input parameters. In parameter studies ridge approximations allow the low-dimensional structure to be exploited, reducing the effective dimension. We introduce a new, fast algorithm for constructing a ridge approximation when the nonlinear function is a polynomial by minimizing the least squares mismatch between the surrogate and the quantity of interest on a given set of inputs. Then, for functions that exhibit this ridge structure, we show how to build quadrature rules that exploit this structure and reduce the cost of high dimensional integration.

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MS54

Dimension Reduction for Remote Sensing and Data Fusion

Remote sensing of vertical profiles of green house gases from satellites and ground based instruments typically results in ill-posed inverse problems where the degrees of freedom of the signal is low and prior information has a significant role. To be able to efficiently extract the information content of the observations, likelihood informed dimension reduction is applied. Further, when observations from different sources are assimilated together, the procedure can be seen as high dimensional time series analysis. If the underlying fields to be modeled are smooth, we can utilize similar dimension reduction techniques. This will result as an efficient Kalman smoother algorithm. The talk will explain the theory behind the algorithms and give application examples in the field of environmental monitoring.

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MS54

Adaptive Dimension Reduction to Accelerate Infinite-dimensional Geometric MCMC

Bayesian inverse problems highly rely on efficient and effective inference methods for uncertainty quantification. Infinite-dimensional MCMC algorithms, directly defined on function spaces, are robust under refinement (through discretization, spectral approximation) of physical models. Recently, a class of algorithms also starts to take advantage of geometric information provided by, for example, quadratic approximation of the parameter-to-observation map so that they are capable of exploring complex probability structures, as frequently arise in UQ for PDE constrained inverse problems. However, the required geometric information is very expensive to obtain in high dimensions. The issue can be mitigated by dimension reduction techniques. By carefully splitting the unknown parameter space into a low-dimensional geometry-concentrated subspace, and an infinite-dimensional geometry-flat subspace, one may then apply geometry-informed MCMC algorithms to the low-dimensional subspace and simpler methods to the infinite-dimensional complement. In this work, we explore randomized linear algebraic algorithms as efficient dimension reducing tools to adaptively obtain low dimensional subspaces. This is applied to speed up particular geometric infinite-dimensional MCMC methods. The speed-up of dimension-reduced algorithms is tested on both a simulation example and a real application in turbulent combustion.

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MS54

Certified Dimension Reduction for Nonlinear Bayesian Inverse Problems

A large-scale Bayesian inverse problem has a low effective dimension when the data are informative only on a low-dimensional subspace of the input parameter space. Detecting this subspace is essential for reducing the complexity of the inverse problem. For example, this subspace can be used to improve the performance of MCMC algorithms and to facilitate the construction of surrogates for expensive likelihood functions. Several different methods have recently been proposed to construct such a subspace—in particular, gradient-based approaches like the likelihood-informed subspace method and the active subspace method, or non-gradient-based methods like the truncated Karhunen-Loeve decomposition. In the context of nonlinear inverse problems, however, these methods are essentially heuristics whose approximation properties are poorly understood. We develop a new method which allows bounding the Kullback-Leibler divergence between the posterior distribution and the approximation induced by certain decompositions. We then identify the subspace that minimizes this bound, and compute it using gradients of the likelihood function. This approach allows the approximation error to be rigorously controlled. A numerical comparison with existing methods favorably illustrates the performance of our new method.

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MS55

Point Cloud Discretization of Fokker-Planck Operators for Committor Functions

The committor functions provide useful information to the understanding of transitions of a stochastic system between disjoint regions in phase space. In this work, we develop a point cloud discretization for Fokker-Planck operators to numerically calculate the committor function, with the assumption that the transition occurs on an intrinsically low-dimensional manifold in the ambient potentially high dimensional configurational space of the stochastic system. Numerical examples on model systems validate the effectiveness of the proposed method.

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MS55

Rare Event Analysis on Random Elliptic PDEs with Small Noise

Partial differential equations with random inputs have become popular models to characterize physical systems with

uncertainty. In this talk, I will present asymptotic rare event analysis for such elliptic PDEs with random inputs. In particular, we consider the asymptotic regime that the noise level converges to zero suggesting that the system uncertainty is low, but does exists. We develop sharp approximations of the probability of a large class of rare events.

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MS55

A Multilevel Approach Towards Unbiased Sampling of Random Elliptic Partial Differential Equations

Partial differential equation is a powerful tool to characterize various physics systems. In practice, measurement errors are often present and probability models are employed to account for such uncertainties. In this paper, we present a Monte Carlo scheme that yields unbiased estimators for expectations of random elliptic partial differential equations. This algorithm combines multilevel Monte Carlo and a randomization scheme proposed by Rhee and Glynn (2012, 2013). Furthermore, to obtain an estimator with both finite variance and finite expected computational cost, we employ higher order approximations.

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MS55

Model Reduction for Diffusion-like Processes near Low-dimensional Manifolds in High Dimensions

We assume we have access to a (large number of expensive) simulators that can return short simulations of high-dimensional stochastic system, and introduce a novel statistical learning framework for learning automatically a family of local approximations to the system, that can be (automatically) pieced together to form a fast global reduced model for the system, called ATLAS. ATLAS is guaranteed to be accurate (in the sense of producing stochastic paths whose distribution is close to that of paths generated by the original system) not only at small time scales, but also at large time scales, under suitable assumptions on the dynamics. We discuss applications to homogenization of rough diffusions in low and high dimensions, as well as relatively simple systems with separations of time scales, and deterministic chaotic systems in high-dimensions, that are well-approximated by stochastic differential equations.

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MS56

Polynomial Approximation of High-dimensional Functions on Irregular Domains

Smooth, high-dimensional functions defined on tensor domains can be approximated using simple orthonormal bases formed as tensor products of one-dimensional orthogonal polynomials. On the other hand, constructing orthogonal polynomials on irregular domains is a difficult and computationally-intensive task. Yet irregular domains arise in many practical problems, including uncertainty quantification, model-order reduction, optimal control and numerical PDEs. In this talk I will discuss the approximation of smooth, high-dimensional functions on irregular domains using a method known as polynomial frame approximation. Importantly, this method corresponds to approximation in a frame, rather than a basis; a fact which leads to several key differences, both theoretical and numerical in nature. However, this method requires no orthogonalization or parametrization of the domain boundary, thus making it suitable for very general domains. I will discuss theoretical results for the approximation error, stability and sample complexity of this algorithm, and show the methods suitability for high-dimensional approximation through independence (or weak dependence) of the guarantees on the ambient dimension d. I will also present several numerical results, and highlight some open problems and challenges.

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MS56

Convergence of Sparse Polynomial Collocation in Infinite Dimensions

Abstract not available at time of publication.

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MS56

Optimal Weighted Least-squares Methods for Ap-

proximation in High Dimension

In arbitrary dimension d, we consider the problem of reconstructing an unknown bounded function u defined on a domain $X \subseteq R^d$ from noiseless or noisy samples of u at n points. We measure the reconstruction error in the $L^2(X, d\rho)$ norm for some probability measure $d\rho$. Given a linear space V_m with $\dim(V_m) \leq n$, we study the weighted least-squares approximation of u from V_m based on independent random samples. We establish results in expectation and in probability for the convergence of weighted least-squares estimators. These results show that for an optimal choice of the sampling measure $d\mu$ and weight function, which depends on V_m and $d\rho$, stability and optimal accuracy of the estimators are achieved under the mild condition that n scales linearly with m, up to an additional logarithmic factor. Afterwards we discuss sampling methods for the efficient generation of independent random samples from the optimal measure $d\mu$, and finally show some numerical results when $d\rho$ is a product measure and V_m are multivariate polynomial spaces.

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MS56

A Domain-decomposition-based Approximation Technique for Convection-dominated PDEs with Random Velocity Fields

We developed a new model-order reduction technique for PDEs with random field input. In our approach, domain decomposition is used to reduce the parametric dimension in local physical domains; proper orthogonal decomposition is used to reduce the degree of freedom along the interfaces and within subdomains, and sparse approximation is used to construct surrogate to the local stiffness matrices obtained from Schur complement. The main advantages of our method are: (i) the complexity of the surrogate model is independent the FEM mesh size (online-offline decomposition); (ii) being able to handle both colored noise and discrete white noise (i.e., piecewise constant random fields); and (iii) promising accuracy in solving convection-dominated transport with random velocity fields.

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MS57

Inferring on the Parameters of a Microscopic Model from the Estimated Parameters of a Macroscopic One

Estimating the unknown parameters of a microscopic, stochastic model from large scale observations poses a number of challenges, and requires the development of new methodological approaches. In the Bayesian statistical framework, stochastic forward models often lead to intractable likelihood densities, making standard statistical computations a challenge. Such models are addressed by Approximate Bayesian Computing (ABC). We propose an alternative approach combining Bayesian statistics and particle techniques for inference beyond the limits of model scales. The viability of the approach is demonstrated on three computed examples describing diffusion, chemical kinetics, and cell culture assay, and a connection with existing ABC methods is discussed.

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MS57

Numerical Posterior Distribution Error Control and Bayes Factors in the Bayesian Uncertainty Quantification of Inverse Problems

In the Bayesian analysis of Inverse Problems most relevant cases the forward maps are defined in terms of a system of (O, P)DE's that involve numerical solvers. These solvers then lead to a numerical (approximated) posterior distribution. Recently several results have been published on the regularity conditions required on such numerical methods to ensure converge of the numerical to the theoretical posterior. However, more practical guidelines are needed. I present some recent results that, by using Bayes Factors, one can see that the numerical posterior tends to the theoretical posterior in the same order as the numerical solver used in the forward map. Moreover, when error estimates are available for the solver we can use a bound on this errors, proven to lead to basically error free posteriors. That is,given that we are observing noisy data, we may tolerate an amount (relative to the data noise) of numerical error in the solver, and end up with a basically error free posterior. In this talkI will show these results, present some examples in ODEs and PDEs and comment on the generalizations to the infinite dimensional setting.

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MS57

Multilevel Sparse Leja Approximations in Bayesian Inversion

The Bayesian inversion of complex, high-dimensional applications is challenging, both mathematically and computationally. In addition, the prior distribution – the known or assumed knowledge about the solution before any measurement data is accounted for – has a large influence on the solution of the inversion, i.e. the posterior distribution. In this talk, we propose an approach to tackle the aforementioned challenges, as follows. We employ multilevel adaptive sparse grid collocation to construct a surrogate of the underlying forward model such that, as we perform

the multilevel decomposition, we sequentially update the prior knowledge. To this end, to discretize the problem's domain, we use a hierarchy of finite elements with a resolution increasing by a constant factor. To discretize the stochastic domain, we use adaptive sparse approximations constructed on weighted Leja sequences. While on the first level we construct the surrogate via discretizing the prior space, starting with the second level we take advantage of the multilevel decomposition and we construct weighted Leja points using the posterior from the previous level as weight function; since sparse grids are defined on tensor-product spaces, we first need to transform these posteriors into separable distributions via e.g., variational Bayes approaches or copula transforms. To obtain a comprehensive overview of our approach, we test it in several problems.

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MS57

Iterative Update of Modeling Error in Computational Inverse Problems

Inverse problems are characterized by their sensitivity to noise in the data. In addition to the exogenous observation noise, errors due to discretization, model uncertainties such as ill-determined model parameters should be taken into account, in particular when the quality of the data is good and the modeling errors dominate. In the Bayesian framework, the mode errors allow a description as random variable with a distribution that can be approximated based on the current information about the unknown interest, such as the prior distribution. In this talk, some recent results concerning iterative updating of the modeling error are discussed. The work is based on collaboration with Daniela Calvetti, Matt Dunlop and Andrew Stuart.

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MS58

Model Error in Co2 Retrievals for the Oco-2 Satellite

The Orbiting Carbon Observatory 2 (OCO-2) collects space based measurements of atmospheric CO2. The CO2 measurements are indirect, the instrument observes radiances (reflected sunlight) over a range of wavelengths and a physical model is inverted to estimate the atmospheric CO2. This inference is in fact an estimation of physical parameters, which can be both biased and overconfident when model error is present but not accounted for. The OCO-2 operational data processing addresses this problem in a few different ways, e.g. with a post-inference bias correction procedure based on ground measurements. This talk will discuss methods to account for informative model error directly in the inversion procedure to lessen bias and provide more reliable uncertainty estimates.

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MS58

Embedded Model Error and Bayesian Model Selection for Material Variability

The advent of fabrication techniques like additive manufacturing has focused attention on the considerable variability of material response due to defects and other microstructural aspects. This variability motivates the development of an enhanced design methodology that incorporates inherent material variability to provide robust predictions of performance. In this work, we develop plasticity models, with calibrated model errors, capable of capturing the range of experimental observations due to material variability using Bayesian inference. The model error is introduced by embedding the modeled stochasticity through calibrated distributions on the physical parameters of the model itself [Sargsyan et al., 2015]. The choice of physical parameters used in such embedding is made using Bayesian model selection method [Verdinelli et al., 1996]. We quantify the aleatory uncertainty present in the experimental observations consisting of high-throughput micro-stress-strain curves of additively manufactured stainless steel. We demonstrate that predicted confidence intervals effectively captures the scatter in the experimentally-observed quantities of interest.

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MS58

A Stochastic Operator Approach to Representing Model Inadequacy

Models are imperfect representations of complex physical processes. Representing the uncertainties caused by using inadequate models is crucial to making reliable predictions. We present a model inadequacy representation in the form of a stochastic operator acting on the state variable and discuss methods of incorporating prior knowledge of model shortcomings and relevant physics. This formulation is developed in the context of an inadequate model for contam-

inant transport through heterogeneous porous media.

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MS58

Physics-constrained Data-driven Modeling of Computational Physics

With the proliferation of high quality datasets, there is a tendency to assume that physical modeling can be replaced by data-driven modeling. In this talk, we show some examples of the limitations of relying solely on data to construct models of physical problems. A pragmatic solution is to combine physics-based models with data-based methods and pursue a hybrid approach. The rationale is as follows: by blending data with existing physical knowledge and enforcing known physical constraints, one can improve model robustness and consistency with physical laws and address gaps in data. This would constitute a data-augmented physics-based modeling paradigm. An approach that introduces physics constraints with statistical inference, machine learning and uncertainty propagation will be introduced. Examples will be presented in applications involving the modeling of fluid flows and molecular dynamics.

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MS59

Calibration, Compensation, Parameter Estimation, and Uncertainty Quantification for Nanoelectrode Array Biosensors

This paper presents the use of a statistical approach to estimate physical/electrochemical parameters of impedance spectroscopy experiments performed with a realistic nanoelectrodes array biosensor platform. The Bayesian estimation methodology is based on the combination of nanobiosensor simulations, performed with the ENBIOS tool, with Markov-Chain Monte Carlo (MCMC) analyses. A simple 1D electrode-electrolyte geometry is first considered as a validation test case, allowing the accurate estimation of Stern layer permittivity and salt concentration, as set by a reference analytical model. Then, full 3D analyses of the nanoelectrodes array system are performed in order to estimate a number of relevant parameters for measurements in electrolyte. Furthermore, moving to more challenging test cases, size/permittivity of microparticles suspended in electrolyte will also be discussed. This methodology allows for the determination of impedance spectroscopy data parameters, and quantification of parameter uncertainties in these multi-variable detection problems. It is thus a very promising approach in order to improve the precision of biosensor measurement predictions, which are intrinsically affected by many parameters.

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MS59

Optimal Multi-level Monte Carlo and Adaptive Grid Refinement for the Stochastic Drift-diffusion-poisson System

In this work, we propose an adaptive multilevel Monte-Carlo algorithm to solve the stochastic drift-diffusion-Poisson system. The method is used to quantify noise and fluctuations in various nanoscale devices, e.g., double-gate MOSFETs and FinFETs. The fluctuation due to the random position and the random number of impurity atoms is a challenging problem and leads to the uncertainty in the device. Here, we use the finite-element method to model the charge transport. In order to analyze the error, we first prove an a-priori error estimate and show that the error converges quadratically. Afterwards, we use an a-posteriori error estimate to define a local error indicator for each element and determine in which part of the domain the error is particularly high and, therefore, more mesh elements are necessary. In the developed technique, in the multilevel Monte-Carlo setting, adaptive mesh refinement according to the error indicator derived is used instead of uniform mesh refinement. For a given error tolerance ϵ, we refine the mesh as long as the discretization error is larger than $\epsilon^2/2$. Then, we define an optimization problem to calculate the optimal number of samples. In other words, the total work is minimized subject to the condition that the statistical error is equal to $\epsilon^2/2$. Compared with uniform mesh refinement, better statistical and discretization error convergence is achieved and lower computational work is obtained.

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MS59

Maximum-principle-satisfying Second-order Intrusive Polynomial Moment Scheme

Using standard intrusive techniques when solving hyperbolic conservation laws with uncertainties can lead to oscillatory solutions as well as non-hyperbolic moment systems. The Intrusive Polynomial Moment (IPM) method ensures hyperbolicity of the moment system while restricting oscillatory over- and undershoots to specified bounds. In this talk, we derive a second-order discretization of the IPM moment system which fulfills the maximum principle. This task is carried out by investigating violations of the specified bounds due to the optimization method as well as the limiter used in the scheme. This investigation gives weaker conditions on the entropy that is used, allowing the choice of an entropy which enables choosing the exact minimal and maximal value of the initial condition as bounds. Solutions calculated with the derived scheme are non-oscillatory while fulfilling the maximum principle. As the scheme is second-order accurate, we are able to heavily reduce the numerical costs.

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MS59

Sensitivity Analysis and High Dimensional Kinetic Equation with Uncertainty

We study the Vlasov-Poisson-Fokker-Planck system with uncertainty and multiple scales. Here the uncertainty, modeled by random variables, enters the solution through different sources, while the multiple scales lead the system to its high-field or parabolic regimes. With the help of proper Lyapunov-type inequalities, under some mild conditions on the uncertainty, the regularity of the solution in the random space, as well as exponential decay of the solution to the global Maxwellian, are established under Sobolev norms, which are uniform in terms of the scaling parameters. These are the first hypocoercivity results for a nonlinear kinetic system with random inputs. Based on the sensitivity analysis in random space, we established the spectral convergence of the generalized Polynomial Chaos stochastic Garlerkin method. We also proved a reduced basis method breaks the curse of dimensionality for several kinetic equations with high dimensional random inputs. Numerical examples is given to verify the properties at the end.

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MS60

An Adaptive Local Reduced Basis Trust-region Method for Risk-averse PDE-constrained Optimization

The numerical solution of risk-averse PDE-constrained optimization problems requires substantial computational effort resulting from the discretization of the underlying PDE in both the physical and stochastic dimensions. To practically solve problems with high-dimensional uncertainties, one must intelligently manage the individual discretization fidelities throughout the optimization iteration. In this work, we combine an inexact trust-region algorithm with the recently developed local reduced basis approximation to efficiently solve risk-averse optimization problems with PDE constraints. The main contribution of this work is a numerical framework for systematically constructing surrogate models for the trust-region subproblem and the objective function using local reduced basis approximations. We demonstrate the effectiveness of our approach through a numerical example.

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MS60

Risk-averse Topology Optimization

Topology optimization is an iterative design process which optimally distributes a volume of material by minimizing an objective and fulfilling a set of constraints. Each iteration step requires a solution of a PDE describing the physics of the problem. The material distribution is represented by using a density field which takes values one if a point is occupied with material and zero otherwise. Regularization techniques ensure the existence of a solution. The density field is obtained by a set of transformations applied on intermediate density like fields. Recently these intermediate fields have been identified to match transformations in nano- and micro-scale manufacturing. These similarities lead to optimized solutions described directly by control parameters supplied to the manufacturing equipment. Imperfections in the production are modeled as additional random fields and random variables affecting the system response directly. The introduction of uncertainties leads to full digitalization of the design-manufacturing chain without any human intervention. However, such a desired scenario increases further the already high computational requirements. Thus, the goal of the presentation is to discuss and to compare different techniques for lowering of the computational burden. The methods transform the initial topology optimization problem in computationally feasible one.

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MS60

Scalable Algorithms and Software for PDE-constrained Optimization under Uncertainty

Optimal control and design of physical systems modeled by partial differential equations (PDEs) is an important goal of many science and engineering applications. Typically, PDE inputs such as model coefficients, boundary conditions and initial conditions are unknown and estimated from noisy, incomplete data. The numerical solution of these problems poses a number of theoretical, algorithmic and software challenges. We begin this talk by introducing risk measures as a means of controlling uncertainty in the model parameters. Second, we review several optimization formulations that enable scalable solution techniques, and outline a few numerical algorithms. Third, we discuss their implementations in the Rapid Optimization Library (ROL). To conclude, we solve risk-neutral and risk-averse PDE-constrained optimization problems using ROL in two application areas: optimal control of thermal fluids and topology optimization of elastic structures.

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MS60

Sparse Solutions in Optimal Control of PDEs with Uncertain Coefficients

Sparse solutions of optimal control problems governed by elliptic PDEs with uncertain coefficients are studied. In applications, regions with nonzero controls can be interpreted as optimal locations for control devices. Two formulations are presented, one where the target is a deterministic optimal control that optimizes the mean control objective, and a formulation aiming at stochastic controls that all share the same sparsity structure. I will focus on the stochastic control problem governed by a linear elliptic PDE with linearly entering infinite-dimensional uncertain parameter field. I propose and analyze a norm reweighting algorithm for the solution of this problem. Combined with low-rank operator approximations, this results in an efficient solution method that avoids iteration over the uncertain parameter space. Numerical examples with the Laplace and Helmholtz PDE operators are presented.

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MS61

An Adaptive Multi-fidelity Metamodel for UQ and Optimization Based on Polyharmonic Spline

Ship hydrodynamic performance is significantly affected by operational and environmental uncertainty, stemming from speed, sea state and wave spectrum parameters, heading. The quantification of the effects of these uncertain parameters on the ship performance (resistance, motions, etc.) is evaluated by coupling hydrodynamic solvers (possibly high-fidelity) with UQ methods. Furthermore, in order to define robust and reliable hull forms, the estimators provided by UQ are included as merit factors in a simulation-based design optimization process. The latter can be computationally very expensive and therefore efficient methodologies for both UQ and optimization are sought after. Here, an adaptive multi-fidelity metamodel (AMFM) is presented to reduce the computational effort while maintaining highly accurate predictions. The AMFM combines the interpolation of high- and low-fidelity solutions based on an ensemble of polyharmonic spline. The metamodel training sets (low- and high-fidelity) are refined based on the scatter in the predictions. A method is presented for selecting adaptively which fidelity needs to increase the training set size. The use of AMFM with UQ and optimization methods is discussed. The proposed AMFM is applied to the UQ and hull form optimization of a destroyer-type ship, subject to uncertain cruise speed, where high- and low-fidelity solutions are provided by RANS and potential-flow solvers, respectively.

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MS61

B-splines on Sparse Grids for Stochastic Collocation

The sparse grid combination technique is an established method to tackle higher-dimensional problems in the context of uncertainty quantification. Classical approaches use combinations of anisotropic full grids with global polynomials as basis functions to approximate quantities of interest or to compute coefficients of the polynomial chaos expansion via pseudo spectral projection. We replaced the global polynomial basis in the sparse grid combination technique by a local B-Spline basis to reduce negative effects of numerical instabilities in the solution on the surrogate. B-Splines do not suffer from Gibb's phenomenon, and their polynomial degree can be chosen arbitrarily depending on the problem at hand to increase the order of convergence. We introduce a not-a-knot B-Spline basis for anisotropic full grids to cope with inaccuracies at the boundary of the stochastic domain. Furthermore, we use established adaptive refinement criteria that are derived from the sparse grid approach to reduce the costs, i.e. the number of forward model runs, for the approximation. Numerical studies demonstrate the effectiveness of this approach compared to common sparse grid methods with various grids based on Clenshaw-Curtis points and Leja sequences as well as to polynomial chaos expansion.

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MS61

Soft Information in Uncertainty Quantifications

We propose a framework for uncertainty quantification based on nonparametric statistical estimation and soft information about shape, support, continuity, slope, location of modes, values, and other properties of the probability density function (pdf) of a response quantity of interest. Using maximum likelihood, maximum entropy, and related criteria, we obtain estimators of such pdfs and establish their strong consistency under mild assumptions and robustness in the presence of model misspecification. We also achieve strong consistency of a rich class of plug-in estimators for modes of pdfs for response quantities. Computations are facilitated by approximation of the nonparametric estimation problems using epi-splines. Specific examples illustrate the framework including an estimator simultaneously subject to bounds on pdf values and its (sub)gradients, restriction to concavity, penalization that encourages lower modes, and imprecise information about the expected value of the response quantity of interest.

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MS61

IGA-based Multi-index Stochastic Collocation

Multi-Index Stochastic Collocation (MISC) is a method of the multi-level family, aimed at reducing costs when repeatedly solving a parametric PDE for UQ purposes by exploiting a hierarchy of discretizations. In this talk, we show how to combine MISC with Isogeometric Analysis (IGA) solvers, leveraging on their tensor-structure. IGA solvers employ splines instead of finite elements to solve PDEs, which enables simpler meshing process, exact geometry representation and high-continuity basis functions.

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MS62

Convergence of Consistent Bayesian Inversion using Surrogates

We summarize a newly developed Bayesian approach to constructing pullback probability measures regularized by prior densities solving stochastic inverse problems. To improve computational efficiency, we investigate the use of surrogate approximations to the parameter-to-observable map at the heart of the inverse problem. We consider the practical conditions required of the surrogate approximations and their refinements such that we can prove the approximate posterior densities converge. The main theoretical result represents a converse to Scheffe's lemma in the context of stochastic inverse problems and requires a generalization of the famous Arzela-Ascoli theorem to certain spaces of discontinuous functions. Numerical results are used to motivate the conceptual issues and highlight the strategy considered in this theoretical approach to proving convergence.

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MS62

Adaptive Sampling for Efficient UQ using Voronoi Piecewise Surrogates

Voronoi Piecewise Surrogate (VPS) models have been recently introduced as a local alternative to standard global surrogate models for Uncertainty Quantification (UQ) in computational simulations. VPS models were demonstrated successful in modeling high-dimensional functions that exhibit discontinuities, without constraining sample locations. In its basic (non-adaptive) version, a VPS model is constructed on a user-defined sampleset. From an implementation perspective, a highly desired feature in a surrogate model is its ability to propose future samples for improving the model accuracy. In this work, we introduce a new adaptive sampling capability of VPS models that caters to both requirements. Our adaptation mechanism relies on information from iteratively-constructed VPS models to generate new samples. We demonstrate the efficiency of adaptive VPS models using a collection of test functions that exhibit different behaviors (e.g. noise, high gradients, and discontinuities). We compare our adaptive VPS model to standard surrogates such as Sparse Grids, and Gaussian Processes.

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MS62

On the Ensemble Propagation for Efficient Uncertainty Quantification of Mechanical Contact Prob-

lems

A new approach called embedded ensemble propagation has recently been proposed to improve the efficiency of sampling-based uncertainty quantification methods on emerging architectures. It consists of simultaneously evaluating a subset of samples of the model, instead of evaluating them individually. This method improves memory access patterns, enables sharing of information from sample to sample, reduces message passing latency, and improves opportunities for vectorization. However, the impact of these improvements on the efficiency of the code depends on its code divergence, whereby individual samples within an ensemble must follow different code execution paths. In this presentation we will show the feasibility of propagating an ensemble through mechanical contact problems, discuss some of the code divergence issues arising in mechanical contact problems where each sample within an ensemble can give rise to a different contact configuration, discuss strategies to manage them, and illustrate them with numerical examples. At the end we will extend these notions to more general non-linear problems.

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MS62

An Ensemble Generation Method for Efficient UQ Based on Local Surrogate Models

Several Uncertainty Quantification (UQ) methods require ensemble propagation of samples for efficient processing on parallel architectures. In this work, we introduce a new ensemble generation capability based on adaptive random sampling. While many methods focus on finding the best way for grouping selected samples into efficient ensemble(s), our approach generates an ensemble of samples from scratch, adding degrees of design freedom. We use adaptive random sampling to iteratively choose samples with best efficiency, while respecting a user-desired accuracy loss tolerance. In each iteration, we construct two Voronoi Piecewise Surrogate (VPS) models to quantify accuracy and cost. VPS models were recently demonstrated successful in modeling high-dimensional functions that exhibit discontinuities, without constraining sample locations. We compare our algorithm to standard grouping techniques built on sparse grids.

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MS63

A Conditional Gaussian Framework for Filtering and Predicting Complex Nonlinear Dynamical Systems

We introduce a conditional Gaussian framework for data assimilation and prediction. Despite the conditional Gaussianity, the dynamics remain highly nonlinear and capture strongly non-Gaussian features such as intermittency and extreme events. The conditional Gaussian structure allows efficient and analytically solvable conditional statistics that facilitates the real-time data assimilation and prediction. The talk will include three applications of such conditional Gaussian framework. In the first part, a physics-constrained nonlinear stochastic model is developed, and is applied to data assimilation and the prediction of the Madden-Julian oscillation with strongly intermittent features. The second part regards the state estimation of multiscale and turbulent ocean flows using noisy Lagrangian tracers. A suite of reduced filters are designed and compared in filtering different features. In the last part of the talk, a brief discussion of applying conditional Gaussian filters to solve high-dimensional Fokker-Planck equation will be included. This method is able to beat the curse of dimensions in traditional particle methods.

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MS63

More Data is not Always Better: Why and How Feature-based Data Assimilation can be Useful

Suppose you are interested in a system that exhibits transitions from one steady state to another. You have a model for this situation and you are also given data. Your goal is to use the data to estimate parameters of your model. You may ask: are data collected during steady state redundant? If so, one may neglect some, or most, of the steady state data and focus on those data collected during the transition periods. We show by numerical examples that this is indeed the case. The solution of a parameter estimation problem that uses only data collected during transition periods is almost identical to the solution of the problem that uses all of the data, but the problem with fewer data is numerically easier to solve. We present these finding using a mass-spring-damper system as a prototypical example, and

also present progress towards a more rigorous framework for such ideas. More generally, we discuss a feature-based approach to parameter estimation. The idea is to identify low-dimensional features within the data and to estimate model parameters based on these features rather than the raw data. This approach can reduce the intrinsic dimension of a parameter estimation problem which makes obtaining its solution numerically feasible.

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MS63

A Class of Nonlinear Filters Induced by Local Couplings

We introduce a class of structure-exploiting nonlinear filters for high-dimensional state-space models with intractable transition kernels. The idea is to transform the forecast ensemble into samples from the current filtering distribution by means of a sequence of local (in state-space) nonlinear couplings computed mostly via low-dimensional convex optimization. This sequence of low-dimensional transformations implicitly approximates the projection of the filtering distribution onto a manifold of sparse Markov random fields (not necessarily Gaussian) and can be carried out with limited ensemble sizes. Many square-root ensemble Kalman filters can be interpreted as special instances of the proposed framework when we restrict our attention exclusively to linear transformations, and when we neglect approximately sparse Markov structure in the filtering distribution. We consider applications to chaotic dynamical systems.

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MS63

Particle Filters for Spatially Extended Systems

Data assimilation is the process of combining mathematical models with collected observations in order to make forecasts and quantify the associated uncertainty. In this talk, we will focus on the sequential nature of many DA problems; this context naturally leads to the repeated application of Bayes formula. The particle filter algorithm is a Monte-Carlo based approach that allows a straightforward numerical implementation of these recursive updates. Particle filters rely on importance sampling combined with a re-sampling step in order to propagate a set of particles forward in time; contrarily to other methods such as the Ensemble Kalman Filter (EnKF), particle filters do not rely on Gaussian assumptions and are asymptotically exact.Although consistent, in order to give reliable results (i.e. avoid collapse), particle filters typically require a number of particles that scale exponentially quickly with the (effective) dimension of the state-space; traditional particle filters are consequently unusable for many large scale applications. To make progress, the spatial decorrelation that is inherent to many applied scenarios has to be exploited through localization procedures. In this talk, we review some of the techniques that have recently been developed for this purpose and propose some new extensions.

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MS64

Bayesian Optimization using Stacked Gaussian Processes

A Bayesian optimization strategy is presented in the context of Stacked Gaussian Processes. StackedGP is a network of independently trained Gaussian processes used to integrate different datasets through model composition. By using analytical first and second-order moments of a Gaussian process with uncertain inputs, approximated expectations of quantities of interests that require an arbitrary composition of functions can be obtained. A StackedGP-based Bayesian optimization is presented in the context of heterogeneous catalysis to propose new materials by accounting for the uncertainty in adsorbed and activation energies.

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MS64

Scalable Methods for Bayesian Optimal Experimental Design, with Applications to Inverse Scattering

Abstract not available at time of publication.

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MS64

Extending the use of Statistical Emulators in Bayesian Experimental Design

The location of high-dimensional Bayesian designs is a computationally challenging task due to the requirement of optimising an expensive and noisy utility function. We tackle this problem through proposing the k-dimensional approximate coordinate exchange algorithm which extends the use of emulators in the search for the optimal design. The chosen emulator is the Gaussian Process where the utility of a given design is interpolated as a function of distance from a training set of designs. We propose an algorithm for training and adaptively augmenting the emulator for the location of efficient Bayesian designs. We compare our algorithm against current best practice, and show that our approach locates highly efficient designs particularly in high dimensional design problems.

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MS64

Towards Exascale Computing: Optimal Parallelization of Experimental Design

Plasma-Wall-Interaction(PWI) related simulations may take days to weeks of simulation-time. It is thus mandatory to utilize the available computational budget efficiently. However, many of the input parameters are uncertain and a proper comparison of the simulation results with experimental data requires the quantification of the uncertainty of the code results as well. Unfortunately the curse of dimension often prohibits a straightforward Monte Carlo sampling of the uncertain parameters. Bayesian Experimental Design together with the use of surrogate models (Gaussian processes) suggests a more efficient approach. Employing the Kullback-Leibler-divergence as utility function we propose an optimized and automated parameter selection procedure for the simulations. The proposed method is applied to PWI-simulations with several uncertain and Gaussian distributed input parameters. New approaches to reduce the wall-clock-time for the optimization as well as the performance of other utility functions are also discussed.

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MS65

Spatiotemporal Pattern Extraction with Operator-valued Kernels

We present a data-driven framework for extracting spatiotemporal patterns generated by ergodic dynamical systems. Our approach is based on an eigendecomposition of a kernel integral operator acting on a Hilbert space of vector-valued observables of the system, taking values in a space of functions (scalar fields) on a spatial domain. This operator is constructed by combining aspects of the theory of operator-valued kernels for machine learning with delay-coordinate maps of dynamical systems. Specifically, delay-coordinate maps performed pointwise in the spatial domain induce an operator acting on functions on that domain for each pair of dynamical states. We show that in the limit of infinitely many delays the resulting kernel integral operator commutes with a Koopman operator governing the evolution of vector-valued observables under the dynamics; as a result, in that limit the recovered patterns lie in simultaneous eigenspaces of these operators associated with the point spectrum of the dynamical system. We present applications of our framework to the Kuramoto-Sivashinsky model, which demonstrate considerable performance gains in efficient and meaningful decomposition over eigendecomposition techniques utlizing scalar-valued kernels.

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MS65

Data-driven Discovery of Dynamical Systems and Uncertainty in Model Selection

Data-driven sparse identification algorithms allow one to select candidate models for governing nonlinear dynamical systems by a Pareto front analysis. Cross validating the model selection process can be performed using AIC or BIC scores for the remaining candidate models. Uncertainty in model parameters can also be cross validated for parametrized systems using group sparsity penalization techniques, thus allowing one to compute UQ metrics for data-driven discovery of nonlinear systems. Our method is demonstrated on a number of physically motivated examples.

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MS65

A Bayesian Topological Framework for the Identification and Reconstruction of Subcellular Motion

Microscopy imaging allows detailed observations of intracellular movements and the acquisition of large data sets that can be fully analyzed only by automated algorithms. This talk will expose a new computational method for the automatic identification and reconstruction of trajectories followed by subcellular particles captured in microscopy image data. The method operates on stacks of raw image data and computes the complete set of contained trajectories. The method engages Bayesian considerations with topological data analysis and makes no assumptions about the underlying dynamics. We test the developed method successfully against artificial and experimental datasets. Application of the method on the experimental data reveals good agreement with manual tracking and benchmarking yields performance scores competitive to the existing state of the art tracking methods.

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MS65

On the Construction of Probabilistic Newton-type Algorithms

It has recently been shown that many of the existing quasi-Newton algorithms can be formulated as learning algorithms, capable of learning local models of the cost functions. Importantly, this understanding allows us to safely start assembling probabilistic Newton-type algorithms, applicable in situations where we only have access to noisy observations of the cost function and its derivatives. This is where our interest lies. We make contributions to the use of the nonparametric and probabilistic Gaussian process models in solving these stochastic optimisation problems. Specifically, we present a new algorithm that unites these approximations together with recent probabilistic line search routines to deliver a probabilistic quasi-Newton approach. We also show that the probabilistic optimisation algorithms deliver promising results on challenging nonlin-

ear system identification problems where the very nature of the problem is such that we can only access the cost function and its derivative via noisy observations, since there are no closed-form expressions available.

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MS66

A Deep Learning Approach in Traffic Prediction for Autonomous Driving

With the development of AI technology, people paid more and more attention to the AI technology which brings real changes to human, especially combined with the traditional industry. Autonomous driving is one of the hottest research areas in the last two years, and it will bring great changes to people's lives. As one of the core issues in the field of automatic driving, prediction of the surrounding vehicles and pedestrians is a very hard problem. We have tried CNN, RNN and other algorithms, and carried out in-depth study. It was applied in the field of automatic driving and achieved good results. In the follow-up study, let us explore together and apply it to real life.

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MS66

Hybrid Data Assimilation for Aerosol Parameter Estimation

Estimation of the parameters which define aerosol distributions, such as the space-time location of the source and the strength and duration of release, is an important problem for applications such as the enforcement of environmental regulations and treaties. The mathematical and computational challenges stem from the sparsity of observations in space and time; the complexity and uncertainty in the nonlinear advection-diffusion-reaction models; and confounding levels of background noise. These factors contribute to an ill-posed and poorly regularized inverse problem. In this talk, we will consider several techniques for parameter estimation in this domain, and focus on a hybrid technique—motivated by the multi-scale structure of the dynamics and sparsity in the data—which aims to reduce the dimensionality of the parameter space and accelerate convergence toward more accurate parameter estimates.

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MS66

Sequential Data Assimilation with Multiple Nonlinear Models and Applications to Subsurface Flow

Complex systems are often described with competing models. Such divergence of interpretation on the system may stem from model fidelity, mathematical simplicity, and more generally, our limited knowledge of the underlying processes. Meanwhile, available but limited observations of system state could further complicate ones prediction choices.Over the years, data assimilation techniques, such as the Kalman filter, have become essential tools for improved system estimation by incorporating both models forecast and measurement; but its potential to mitigate the impacts of aforementioned model-form uncertainty has yet to be developed. Based on an earlier study of Multi-model Kalman filter, we propose a novel framework to assimilate multiple models with observation data for nonlinear systems, using extended Kalman filter, ensemble Kalman filter and particle filter, respectively. Through numerical examples of subsurface flow, we demonstrate that the new assimilation framework provides an effective and improved forecast of system behavior.

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MS66

Probabilistic Machine Learning for Fluid Flows

Previous works have used machine learning to construct data-driven models for predicting various quantities such as turbulent stresses, sub-grid-scale scalar fluxes, and wall-shear stresses in turbulent flows. However, it is desirable to have quantified uncertainties built in such predictions, which are unfortunately lacking in most existing machine learning techniques. We used Bayesian neural networks (BNN) and direct numerical simulation datasets to construct data-driven turbulent constitutive models to predict turbulent stresses from mean flow field variables with quantified uncertainties. The promising results demonstrate that BNN has great potential in science and engineering applications.

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MS67

Graph-based Bayesian Learning: Continuum Lim-

its and Algorithms

The principled learning of functions from data is at the core of statistics, machine learning and artificial intelligence. The aim of this talk is to present some new theoretical and methodological developments concerning the graph-based, Bayesian approach to semi-supervised learning. I will show suitable scalings of graph parameters that provably lead to robust Bayesian solutions in the limit of large number of unlabeled data. The analysis relies on a careful choice of topology and in the study of the the spectrum of graph Laplacians. Besides guaranteeing the consistency of graph-based methods, our theory explains the robustness of discretized function space MCMC methods in semi-supervised learning settings.

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MS67

Conditional Density Estimation, Filtering and Clustering using Optimal Transport

A new non-parametric procedure for the estimation and simulation of conditional probability density $p(x|z)$ is presented. The procedure originates from a data based formulation of the Wasserstein barycenter problem and has the byproduct of removing the effect of undesired covariates from the dataset under consideration. This approach is computationally efficient by means of a low rank tensor factorization and it naturally embeds a Bayesian clustering procedure to be used when only few to no points of x are available for a given z. The methodology is illustrated through examples that include the explanation of variability of ground temperature across the continental United States and the prediction of book preference among potential readers.

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MS67

Dimension Reduction in Optimization-based Sampling

Markov chain Monte Carlo (MCMC) relies on efficient proposals to sample from a target distribution of interest. Recent optimization-based MCMC algorithms for Bayesian inference, e.g. randomize-then-optimize (RTO), repeatedly solve optimization problems to obtain proposal samples. We interpret RTO as an invertible map between two random variables and find that this mapping *preserves* the value of the random variables along many directions. This is an alternative usage of dimension reduction that corresponds to weaker requirements on the selected subspaces.

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MS68

Modeling Rare Events in Complex Systems

I will discuss numerical methods for the study of barrier-crossing events, particularly the string method, and present some applications including transitions in Kuroshio, the wetting transition on patterned solid surface, the isotropic-nematic transition of liquid crystal.

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MS68

A Laguerre Spectral Minimum Action Method for Finding the Most Probable Path

Minimum action method (MAM) is a powerful mathematical tool for computing phase transition phenomena in many noise-driven dynamical systems. Theoretically, the transition time is infinity when noise amplitude takes limit to zero. There exist several approaches to handle the infinite long transition time, e.g. taking a finite but large transition time, using geometric MAM, determining an optimal finite transition time based numerical resolution. In this talk, we introduce another approach, a Laguerre spectral MAM, to handle this problem. This method has several special properties which will be demonstrated by applying it to several nonlinear ODE systems and PDE systems.

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MS68

Minimum Action Method for Systems with Delays

In this work, we develop an hp-adaptivity strategy for the minimum action method (MAM) using a posteriori error estimate and generalize it to deal with systems with delays. MAM plays an important role in minimizing the Freidlin-Wentzell action functional, which is the central object of the Freidlin-Wentzell theory of large deviations for noise-induced transitions in stochastic dynamical systems. We will demonstrate the effectiveness of our method for systems with or without delays.

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MS68

An Improved Adaptive Minimum Action Method

for Non-gradient System

In this talk, I introduce two improvements on the minimum action method(MAM). The first one is to handle the numerical issue of grid points tangling around the saddle point for a large time interval. The original monitor function in the adaptive MAM is updated and linked to the drift vector only so that the numerical derivative on the path is now unnecessary. The improved aMAM has a better robustness. The second one is on the MAM departing from a stable limit cycle, in which the optimal path has an infinite length. By constructing a quadratic solution of the quasi-potential on the limit cycle from the linearized HJB equation, we run the MAM only from a thin tube around the cycle so that the optimal path is truncated to be finitely long. The quadratic solution in need is solved by an efficient numerical method for the underlying Ricatti equation. This is joint work with Yiqun Sun and Ling Lin. The HK GRF 11304715 and 11337216 is acknowledged.

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MS69

Computational Optimal Design of Random Rough Surfaces in Thin-film Solar Cells

Random rough textures can increase the absorbing efficiency of solar cells by trapping the optical light and increasing the optical path of photons, and in turn increases the effectiveness of solar panels. In this talk, I will briefly describe the mechanism and the mathematical modeling of thin film solar cells to start with. Then I will describe how to use mathematical shape control methods to optimally design of random rough surfaces in thin-film solar cells. Finally I will use numerical experiments to show that optimally obtained random textures yield an enormous absorption enhancement, and thus increase the solar panel's energy efficiency.

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MS69

Sparse Grid Quadratures from Conformal Mappings

In this talk we describe the extension of quadrature approximations, built from conformal mapping of interpolatory rules, to sparse grid quadrature in the multidimensional setting. In one dimension, computation of an integral involving an analytic function using these transformed quadrature rules can improve the convergence rate by a factor approaching $\pi/2$ versus classical interpolatory quadrature. For the computation of high-dimensional integrals with analytic integrands, we implement the transformed quadrature rules in the sparse grid setting, and we show that in certain settings, the convergence improvement can be exponential with growing dimension. Numerical examples demonstrate the benefits and drawbacks of the approach, as predicted by the theory.

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MS69

Unified Null Space Conditions for Sparse Approximations via Nonconvex Minimizations

This talk is concerned with sparse polynomial approximation via compressed sensing approach. Nonconvex minimizations are generally closer to l_0 penalty than l_1 norm, thus it is widely accepted that they are able to enhance the sparsity and accuracy of the approximations. However, the theory verifying that nonconvex penalties are as good as or better than l_1 minimization in uniform, sparse reconstruction has not been available beyond a few specific cases. We aim to fill this gap by establishing new recovery guarantees through unified null space properties that encompass most of the currently proposed nonconvex functionals in the literature. These conditions are less demanding than or identical to the standard null space property, the necessary and sufficient condition for l_1 minimization.

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MS69

A Generalized Sampling and Weighted Approach for Sparse Approximation of Polynomial Chaos Expansions

We consider the sampling stretagy of for sparse recovery of polynomial chaos expansions via compressed sensing. In particular, we propose a general framework that sampling with respect to the (weighted) pluripotential equilibrium measure of the domain, and subsequently solves a weighted least-squares problem. The framework covers both the bounded and unbounded cases. We also discuss a potential application of this approach – handling arbitrary polynomical choas expansions.

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MS70

Multifidelity Robust Optimization

This work presents a multifidelity framework for optimization under uncertainty. Designing robust systems can be computationally prohibitive due to the numerous evaluations of numerical models required to estimate system level statistics at each optimization iteration. We propose a multifidelity Monte Carlo approach combined with information

reuse to estimate the first and second moments of the system outputs. The method uses nested control variates to exploit multiple fidelities and information from previous optimization iterations in order to reduce the variance in the moment estimates and the computational cost as compared to standard Monte Carlo simulation.

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MS70

Uncertainty Quantification via a Bi-fidelity Low-rank Approximation Technique

The use of model reduction has become widespread as a means to reduce computational cost for uncertainty quantification of PDE systems. In this work, we presenta model reduction technique that exploits the low-rank structure of the solution of interest, when exists, for fast propagation of high-dimensional uncertainties. To construct this low-rank approximation, the proposed method utilizes models with lower fidelities (hence cheaper to simulate) than the intended high-fidelity model. After obtaining realizations to the lower fidelity models, a set of reduced basis and an interpolation rule are identified and applied to a small set of high-fidelity realizations to obtain this low-rank, bi-fidelity approximation. In addition to the construction of this bi-fidelity approximation, we present convergence analysis and numerical results.

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MS70

Adaptive Refinement Strategies for Multilevel Polynomial Expansions

In the simulation of complex physics, multiple model forms of varying fidelity and resolution are commonly available. In computational fluid dynamics, for example, common model fidelities include potential flow, inviscid Euler, Reynolds-averaged Navier Stokes, and large eddy simulation, each potentially supporting a variety of spatio-temporal resolution/discretization settings. While we seek results that are consistent with the highest fidelity, the computational cost of directly applying UQ in high random dimensions quickly becomes prohibitive. In this presentation, we focus on the development and deployment of multilevel-multifidelity algorithms that adaptively fuse information from multiple model fidelities and resolutions in order to reduce the overall computational burden. In particular, we focus on forward uncertainty quantification using multilevel emulator approaches that employ compressed sensing and tensor trains to exploit sparse and low rank structure. Several approaches for adaptively allocating samples across levels will be explored and compared, based on deployments to both standard model problems and engineered aerodynamic systems.

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MS70

A Multi-fidelity Stochastic Collocation Method for Time-dependent Problems

In this talk, we shall discuss a collocation method with multi-fidelity simulation models to efficiently reconstruct the time trajectory of time-dependent parameterized problems. By utilizing the time trajectories of low/high-fidelity solutions to construct the approximation space, this method is demonstrated to offer two substantial advantages: (1) it is able to produce more accurate results with a limited number of high-fidelity simulations; (2) it avoids instability issues of time-dependent problems due to the nonintrusive nature. We also provide several numerical examples to illustrate the effectiveness and applicability of the method.

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MS71

Selection, Calibration, and Validation of Models in the Presence of Uncertainty: Applications to Modeling Tumor Growth

The development of predictive computational models of tumor growth is faced with many formidable challenges. Some of the most challenging aspects is to rigorously account for uncertainties in observational data, model selection, and model parameters. In this work, we present a set of mathematical models for tumor growth, including reaction-diffusion and phase-fields models, with and without mechanical deformation effects, and models for radiation therapy. The observational data is obtained from quantitative magnetic resonance imaging data of a murine model of glioma, with X-ray radiation administered in the middle of the experimental program. The mathematical models are based on the balance laws of continuum mixture theory, particularly mass balance, and from accepted biological hypotheses on tumor growth. The Occam Plau-

sibility Algorithm (OPAL) is implemented to provide a Bayesian statistical calibration of the model classes, as well as the determination of the most plausible models in these classes relative to the observational data, and to assess model inadequacy through statistical validation processes. The results of the analyses through suggest that the general framework developed can provide a useful approach for predicting tumor growth and radiation effects. Acknowledgments We thank the Center Prevention Research Institute of Texas (CPRIT) for funding through RR160005, and the National Cancer Institute for funding through U01CA174706 and R01CA186193.

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MS71

Dynamic Bayesian Influenza Forecasting in the United States with Hierarchical Discrepancy

Timely and accurate forecasts of seasonal influenza would assist public health decision-makers in planning intervention strategies, efficiently allocating resources, and possibly saving lives. For these reasons, influenza forecasts are consequential. Producing timely and accurate influenza forecasts, however, have proven challenging due to noisy and limited data, an incomplete understanding of the underlying disease transmission process, and the mismatch between the disease transmission process and the data-generating process. In this talk I will introduce a dynamic Bayesian (DB) flu forecasting model that exploits model discrepancy (i.e., the mismatch between the underlying disease transmission model and the data) through a Bayesian hierarchical model. The DB model allows forecasts of partially observed flu seasons to borrow discrepancy information from previously observed flu seasons. We demonstrate the DB's flu forecasting capabilities by comparing the DB model to leading real-world competitors.

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MS71

Conditioning Multi-model Ensembles for Disease Forecasting

The impact of model errors can be reduced by using an ensemble of models and weighing them differentially, conditional on historical data. This is called model averaging. Starting from an ensemble of equally weighted models, we describe a sequential algorithm that updates the weights conditional on time-series data. The method can accommodate black-box models which provide temporal forecasts as distributions. The method assumes that forecasts are Gaussians, and is a shortcoming of the algorithm. We illustrate this method with an ensemble of disease models, using data on influenza outbreaks in the US.

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MS71

Multi-physics Model Error Calibration

Discrepancy between model prediction and physical observation can be attributed to errors in modelling the system, as well as measurement errors in the experiments. The Kennedy-O'Hagan framework has been usually adopted to estimate model discrepancy in static systems. However, this approach cannot be directly implemented in the case of transient multi-physics models, where an error in modelling one of the constituent disciplines would lead to errors in the outputs of other disciplinary models, and these errors would accumulate in time. In this study, we treat the errors in each constituent discipline as external inputs to the corresponding governing equation. These errors are treated as system states, and are estimated along with the other states corresponding to the original model, using Bayesian state estimation, leading to the estimation of modelling errors as well as discrepancies in all the system states. We illustrate this methodology using a flexible panel subjected to hypersonic air flow and experiencing flow-induced pressure loads and heating. We solve the nonlinear state estimation problem using a sampling-based state estimation method, and address the issues of identifiability, variance reduction, and discrepancy source identification.

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MS72

A Bayesian Approach to Quantifying Uncertainty Divergence Free Flows

We treat the statistical regularization of the ill-posed inverse problem of estimating a divergence free flow field u from the partial and noisy observation of a passive scalar ?. Our solution is Bayesian posterior distribution, a probability measure which precisely quantifies uncertainties in u once one specifies models for measurement error and prior knowledge for u. We present some of our recent work which analyzes both analytically and numerically. In particular we discuss some Markov Chain Monte Carlo (MCMC) algorithms which we have developed and refined to effectively sample from . This is joint work with Jeff Borggaard and Justin Krometis

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MS72

Uncertainty Quantification for the Boltzmann - Poisson System

We study the uncertainty quantification for a Boltzmann-Poisson system that models electron transport in semiconductors and the physical collision mechanisms over the charges. We use the stochastic Galerkin method in order to handle the randomness associated to the problem. The main uncertainty in the Boltzmann equation is knowing the initial condition for a large number of particles, which is why the problem is formulated in terms of a probability density in phase space. The second source of uncertainty in the Boltzmann-Poisson problem, directly related to its quantum nature, is the collision operator, as its structure in this semi-classical model comes from the quantum scattering matrices operating on the wave function associated to the electron probability density. Additional sources of uncertainty are transport, boundary data, etc. In this study we choose the energy as a random variable, as it is a crucial variable in the problem that determines both the collision (given by energy and momentum conservation) and transport (via the wave group velocity), whose balance defines the Boltzmann equation. The dimensional cost is intended to be kept minimal, as the energy band is a scalar function of the momentum.

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MS73

Reduced Basis Approach using Sparse Polynomial Chaos Expansions in Computational Fluid Dynamics Applications

One approach to propagate uncertainties in engineering systems is using polynomial chaos expansions. A fundamental, well-known, limitation of polynomial chaos is the curse-of-dimensionality; namely the computational cost grows dramatically with the number of input uncertainties. In this talk, a two-stage non-intrusive uncertainty quantification method is presented in order to address this issue. First, an optimal stochastic expansion, i.e. made of very few basis functions, is derived using proper orthogonal decomposition on a coarse discretization. It is further combined with an adaptive sparse polynomial chaos algorithm in order to construct the covariance matrix at low cost and thus significantly speed up the convergence of the method. Second, the optimal stochastic basis is utilized to expand the stochastic solution on a fine discretization and derive the statistical moments. A practical engineering problem is studied in order to illustrate and quantify the resulting computational savings over more traditional methods for uncertainty quantification in computational fluid dynamics. It consists of an airfoil operating at transonic flow condition, and subject to geometrical and operational uncertainties. It is shown that the proposed two-stage uncertainty quantification method is able to predict statistical quantities with little loss of information and at a cheaper cost than other state-of-the-art techniques.

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MS73

Quantifying Structural Uncertainty in Reynolds-averaged Navier-stokes Turbulence Models for Simulations of Heat Exchangers

Reynolds-averaged Navier-Stokes (RANS) simulations are commonly used for engineering design and analysis of turbulent flow and heat or scalar transport. An important limitation is that the turbulence and turbulent flux models can introduce considerable uncertainty in predictions for complex applications. To enable robust design and optimization based on imperfect RANS results, the objective of this study is to establish a model-form uncertainty quantification method for turbulent scalar flux models. The proposed framework addresses uncertainty in the scalar flux magnitude and direction. First, the method solves a transport equation for the flux magnitude derived from classic second-moment closures, which introduces a dependency of the magnitude on the direction. Second, two different approaches for varying the scalar flux direction are explored: (1) the monotonicity of the scalar flux production term with respect to the flux direction is analyzed, and an algorithm to explore directions that increase or decrease the production is designed; (2) it is assumed that scalar transport is most effective when the flux vector is normal to the local shear plane, and a function to rotate the vector toward that orientation is constructed. Both strategies are applied to a pin-fin heat exchanger for which large-eddy simulation data is available for validation. The results show promising capabilities to bound predictions for the overall heat transfer rate and some local key flow features.

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MS73

Multilevel and Multi-index Sampling for the Forward Propagation of Many Uncertainties in Industrial Applications

Computational models in science and engineering are subject to uncertainty, that is present under the form of uncertain parameters or model uncertainty. Any quantity of interest derived from simulations with these models will also be uncertain. The efficient propagation of the uncertainties is often the computational bottleneck in other UQ problems, such as robust optimisation and risk analysis. The Monte Carlo method is the method of choice to deal with these many uncertainties. However, the plain Monte

Carlo method is impractical due to its expense. We investigate how extensions of the Monte Carlo method, such as Multilevel Monte Carlo and Multi-Index Monte Carlo, and their respective Quasi-Monte Carlo variants, can be used efficiently to solve uncertainty quantification problems in real engineering applications.

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MS73

Robust PDE Constrained Optimization with Multilevel Monte Carlo Methods

We consider PDE constrained optimization problems where the partial differential equation has uncertain coefficients modeled by means of random variables or random fields. We wish to determine a robust optimum, i.e., an optimum that is satisfactory in a broad parameter range, and as insensitive as possible to parameter uncertainties. To that end we optimize the expected value of a tracking type objective with an additional penalty on the variance of the state. The gradient and Hessian corresponding to such a cost functional also contain expected value operators. Since the stochastic space is often high dimensional, a multilevel (quasi-) Monte Carlo method is presented to efficiently calculate the gradient and the Hessian. The convergence behavior is illustrated using a gradient and a Hessian based optimization method for a model elliptic diffusion problem with lognormal diffusion coefficient and optionally an additional nonlinear reaction term. The evolution of the variances on each of the levels during the optimization procedure leads to a practical strategy for determining how many and which samples to use. We also investigate the necessary tolerances on the mean squared error of the estimated quantities. Finally, a practical algorithm is presented and tested on a problem with a large number of optimization variables and a large number of uncertainties.

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MS74

Adaptive Low-rank Separated Representations Based on Mapped Tensor-product B-splines

There is a great need for robust, efficient, and accurate surrogate modeling techniques throughout a plethora of topics in the field of Uncertainty Quantification. Separated Representations (SR) provide an excellent tool for constructing such surrogate models exhibiting rank sparsity with respect to a tensor-product basis. Moreover, there are a variety of available techniques for determining the corresponding expansion coefficients including alternating least-squares routines or compressive sensing. Despite the assortment of algorithms available for the SR construction, the underlying expansion generally employs orthogonal polynomials which are globally differentiable. However, many physical phenomena exhibit localized features or potentially discontinuous regions, due to e.g. bifurcations, for which global polynomials are poor approximants. As a remedy, we utilize non-uniform, tensor-product B-splines where continuity can be iteratively adapted and optimized to accurately represent these non-smooth or localized features. Additionally, these discontinuous regions are not necessarily axis-aligned. Therefore, we introduce a geometric mapping from a Euclidean parametric domain where the tensor-product B-splines are defined. These splines are then mapped to the physical domain where the data exists. This mapping in turn can be optimized, providing the necessary ingredient for a method capable of accurately representing these non axis-aligned discontinuities and bifurcations.

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MS74

Propagating Fuzzy Uncertainties with Hierarchical B-splines on Sparse Grids

Fuzzy logic is a way of describing uncertainties in parameters. In contrast to probabilistic approaches, it is often used to reflect epistemic uncertainties. Zadeh's well-known extension principle can be applied to propagate uncertainty in the input parameters to the output of an objective function. Unfortunately, it requires the solution of a number of global optimization problems. In settings with expensive objective functions, the large amount of function evaluations required by optimization algorithms quickly becomes prohibitively expensive. We follow the approach proposed by Klimke and replace the objective function by a sparse grid surrogate that can be evaluated very cheaply. Sparse grids cope with the curse of dimensionality to some extent allowing moderately high numbers of input parameters. However, only piecewise linear and global polynomial basis functions have been studied so far, both of which have drawbacks. Instead, we propose to use B-splines for the sparse grid basis. In this talk, we will show that the advantages of the new method are three-fold: First, B-splines display higher numerical orders of convergence than piecewise linear functions. Second, B-splines enable gradient-based optimization, as B-splines are in general continuously differentiable and gradients of the B-spline interpolants are explicitly known. Third, we show that it is possible to employ spatial adaptivity to resolve local features of the objective function.

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MS74

IsoGeometric Splines for Smoothing on Surfaces

We propose an Isogeometric approach for smoothing on surfaces, namely estimating a function starting from noisy

and discrete measurements. More precisely, we aim at estimating functions lying on a surface represented by NURBS, which are geometrical representations commonly used in industrial applications. The estimation is based on the minimization of a penalized least-square functional. The latter is equivalent to solve a 4th-order Partial Differential Equation (PDE). In this context, we use Isogeometric Analysis (IGA) for the numerical approximation of such surface PDE, leading to an IsoGeometric Smoothing (IGS) method for fitting data spatially distributed on a surface. Indeed, IGA facilitates encapsulating the exact geometrical representation of the surface in the analysis and also allows the use of at least globally C^1-continuous NURBS basis functions for which the 4th-order PDE can be solved using the standard Galerkin method. We show the performance of the proposed IGS method by means of numerical simulations and we apply it to the estimation of the pressure coefficient, and associated aerodynamic force on a winglet of the SOAR space shuttle.

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MS74

Minimum Spanning Trees and Support Vector Machines for High-dimensional and Discontinuous Spline-based Surrogate Models

A novel approach for forward propagation of uncertainties through models is proposed for the case of discontinuous model responses in high-dimensional spaces. Traditional methods, such as generalised polynomial chaos (gPC), fail when the quantity of interest depends discontinuously on the input parameters. Adaptive sampling methods exist, but the number of sampling points needed for producing accurate solutions is still intractable for complex engineering problems. As a remedy we invented a Minimum Spanning Tree based sampling algorithm, which searches for important features in the response adaptively. A key ingredient of the proposed method, is the decomposition of the random space, by means of a machine learning algorithm (SVM). The samples are classified based their response values, and the SVM searches for a hypersurface, which separates the classes. This classification boundary serves as an approximation of the discontinuity locations in the random space. The domain is cut along the classification boundary and local approximations are constructed on each of the sub-domains. Splines are used for constructing the local approximations. The combination of adaptive sampling, random space decomposition and splines, ensures an approximation without the appearance of Gibbs phenomena, while producing accurate solutions. The proposed method uses many fewer samples than any other adaptive UQ method in literature.

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MS75

Matrix Decomposition Algorithms for Large-scale Data Compression

When working with large ensembles of large-scale PDE solutions, the cost of both storing and post- processing the relevant data can quickly become prohibitive. To mitigate this problem, we present a variety of low-rank matrix decomposition algorithms, demonstrating their utility in generating multi-fidelity approximations using only a fraction (about 5-10 percent) of the original data. In particular, we examine methods which minimize the number of passes one must make over the solution ensembles. These methods include the interpolative decomposition (ID) and two flavors of randomized singular value decomposition algorithms. In all of these algorithms applied to large-scale computational fluid dynamics data, we manage to limit the number of passes required over the data to two and achieve accuracy up to 2-3 digits.

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MS75

Towards Reduced Order Modeling of Liquid-fueled Rocket Combustion Dynamics

Combustion instability in liquid rocket engines (LRE) is an extremely complex phenomenon, with strongly stochastic and nonlinear physics, and time and length scales that range over many orders of magnitude. Though modern computational capability has demonstrated the potential to beyond the empirically-based design analyses of the past, high-fidelity simulations of full-scale combustors remain out of reach, and will continue to be out of reach for engineering work flows, even on Exascale computers. While individual LES simulations of combustion instability in laboratory-scale combustors are relatively routine [Harvazinski et al., Physics of Fluids, 2015], full-scale rocket engine simulations remain too computationally intensive for design applications. Our goal is to address the gap that exists between the high-fidelity simulations of small and simplified geometries and the need for computations of large and complicated domains through reduced order modeling (ROM) for efficient and accurate predictions of combustion instability in LRE. This work will present progress towards the overall goal, and will detail the development of reduced-order models (ROMs) using adaptive bases and stabilized, data-driven techniques for closure. Results will highlight applications of the these ROMs on laboratory-scale LREs. The developed ROMs will be integrated and coupled together in a multi-fidelity framework to model combustion instabilities in the full LRE system.

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MS75

Data-driven Reduced Order Modeling for High Fidelity Simulations of Wind Plants

Exascale computing resources will enable unprecedented accuracy in high-fidelity simulations of turbulent flow within wind plants. These simulations will reveal new insights into complex flow physics, but are too computationally expensive for use in design optimization, controls, or uncertainty quantification (UQ). Data-driven reduced order modeling techniques provide a mathematically rigorous pathway for encapsulating high-fidelity physical insights into low-order surrogate models suitable for controls and UQ. We demonstrate a linear parameter varying (LPV) approach in conjunction with dynamic mode decomposition (DMD) to derive a data-driven low-order linear state space model that preserves input-output relationships. The LPV-DMD model can be used to assess uncertainty in the input-output relationship between turbine controls and power outputs given uncertainty in a model parameter like the LES Smagorinsky coefficient or surface roughness. The high-fidelity snapshots used in the decomposition are obtained from Nalu, a large eddy simulation (LES) framework developed for exascale computing. Additionally, we discuss two extensions to the LPV-DMD tool: streaming DMD where the decomposition is performed in situ in the LES code, and controller design for real-time control of wind plants using data-driven insights from the high-fidelity simulations.

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MS75

Sampling Techniques for Stochastic Economic Dispatch of Large Electrical Grids

As the penetration of renewable energy sources, e.g. wind and solar, into the power grid increases, tools used for capacity and transmission expansion planning must adapt to ensure reliable service at a low cost. Reliability is a product of not only planning, but also the inclusion of reserve generation. However, as the percentage of power supplied to the grid by renewables grows, common practices for including reserves will become increasingly impractical. Exascale computing capabilities will provide a powerful tool to foresee and address reliability problems during the capacity and transmission expansion planning process by enabling the use of higher fidelity mathematical models (e.g. AC optimal power flow) and including explicit representations of uncertainty. One such representation is the sample average approximation (SAA) of the two-stage stochastic optimization problem, which relies on approximating mathematical expectations via sampling. Input samples, also called scenarios, for the SAA must be chosen carefully: e.g. scenarios based on random sampling are not necessarily adequate tests of grid robustness, often lacking events such as large ramps in generation. We develop a method for building scenarios based on importance sampling and the solution of many surrogate models with simplified physics and statistics. The results show improved convergence to the expectation in the SAA and cheaper, yet robust economic dispatch decisions.

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MS76

On the Stability and the Uniform Propagation of Chaos Properties of Ensemble Kalman-Bucy Filters

The Ensemble Kalman filter is a sophisticated and powerful data assimilation method for filtering high dimensional problems arising in fluid mechanics and geophysical sciences. This Monte Carlo method can be interpreted as a mean-field McKean-Vlasov type particle interpretation of the Kalman-Bucydiffusions. Besides some recent advances on the stability of nonlinear Langevin type diffusions withdrift interactions, the long-time behaviour of models with interacting diffusion matrices and conditional distribution interaction functions has never been discussed in the literature. One of the main contributions of the talk is to initiate the study of this new class of models The talk presents a series of newfunctional inequalities to quantify the stability of these nonlinear diffusion processes. The second contribution of this talk is to provide uniform propagation of chaos properties as well as Lp-mean error estimates w.r.t. to the time horizon.

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MS76

Multilevel Monte Carlo for Data Assimilation

Bayesian inference provides a principled and well-defined approach to the integration of data into an a priori known distribution. The posterior distribution, however, is known only point-wise (possibly with an intractable likelihood) and up to a normalizing constant. Monte Carlo methods have been designed to sample such distributions, such as Markov chain Monte Carlo (MCMC) and sequential Monte Carlo (SMC) samplers. Recently, the multilevel Monte Carlo (MLMC) framework has been extended to some of these cases, so that approximation error can be optimally balanced with statistical sampling error, and ultimately the Bayesian inverse problem can be solved for the same asymptotic cost as solving the deterministic forward problem. This talk will concern the recent development of MLMC data assimilation methods, which combine dynamical systems with data in an online fashion, including ML particle filters and ensemble Kalman filters.

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MS76

Convergence Analysis of Ensemble Kalman Inversion

The ideas from the Ensemble Kalman Filter introduced by Evensen in 1994 can be adapted to inverse problems by introducing artifical dynamics. In this talk, we will discuss an analysis of the EnKF based on the continuous time scaling limits, which allows to derive estimates on the long-time behavior of the EnKF and, hence, provides insights into the convergence properties of the algorithm. In particular, we are interested in the properties of the EnKF for a fixed ensemble size. Results from various numerical experiments supporting the theoretical findings will be presented.

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MS76

Long-time Stability and Accuracy of Interacting Particle Filters

In a nonlinear setting the filtering distribution can be approximated via the empirical measure provided that an ensemble of samples is available. A computationally feasible option to generate these particles is to define an appropriate modified evolution equation that describes the dynamics of the particles with respect to the incoming data. The most famous example of such interacting particle filter formulations is the ensemble Kalman-Bucy filter (EnKBF). Although it works remarkably well in practice its success is not well understood from a mathematical point of view. In particular, the long time behavior of the EnKBF far from the asymptotic limit is of interest. In a recent study [de Wiljes, Reich, Stannat, Long-time stability and accuracy of the ensemble Kalman-Bucy filter for fully observed processes and small measurement noise, `https://arxiv.org/abs/1612.06065`] we were able to derive stability and accuracy results for a specific variant of the EnKBF. More specifically we were able to derive lower and upper bounds for the empirical covariance matrix for a fully observed system and a finite number of particles. Further uniform-in-time stability and accuracy results, such as control over the path wise estimation error, were show for the considered EnKBF. Inspired by the EnKBF we also explore more general interacting particle filter formulations that allow to overcome weaknesses of the EnKBF as well as drawbacks of classical sequential resampling schemes.

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MS77

Experimental Design in Diffuse Tomography

This talk considers two diffuse imaging modalities: electrical impedance tomography and thermal tomography. The former aims at reconstructing the conductivity distribution inside a physical body from boundary measurements of current and voltage, whereas the goal of the latter is to deduce information about the internal structure of a physical body from time-dependent temperature measurements on its boundary. In practice, such measurements are performed with a finite number of electrodes or with a finite number of heater elements and temperature sensors. This work considers finding optimal positions for the electrodes in electrical impedance tomography and optimal time-dependent heating patterns for the heater elements in thermal tomography. The goal is to place the electrodes and choose the heating patterns so that the posterior distrbution for the (discretized) parameters of interest is as localized as possible under physically reasonable restrictions on the measurement setup.

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MS77

Planning Sensitivity Tests using Mutual Information

Sensitivity testing involves exposing experimental units to various levels of a stimulus (e.g., heat, impact, voltage) to ascertain population sensitivity to the stimulus. Outcomes are binary and usually modeled with a logistic or probit GLM. In this talk, we describe sequential Bayesian sensitivity tests using mutual information as a design criterion. We also numerically illustrate how sequential D-optimal sensitivity tests, like the Neyer and 3pod methods, have Bayesian interpretations.

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MS77

Bayesian Design for Stochastic Models with Appli-

cation to Models of Infectious Disease Dynamics

We will present recently-developed methods for efficient Bayesian experimental design using Approximate Bayesian Computation. This includes methods for evaluation of the utility, and search across the design space. The application of this framework to stochastic models, and in particular to the design of group dose-response studies in the presence of transmission will be explored.

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MS77

Optimal Design of High-speed Wind Tunnel Instrumentation for Aero-thermal-structural Model Calibration

Modeling the coupled aero-thermal-structural response of a panel subjected to high-speed flight environment is a challenging task. Improving the model prediction confidence with data is complicated by the substantial cost of wind tunnel tests and experimental limitations. Therefore, it is critical to optimally design tests that provide the most informative data possible. Maximum expected information gain is used to determine the instrumentation locations for calibration data on rigid wind tunnel specimen representative of a deformed panel under loading conditions that induce aerothermoelastic coupling. Previous results from Bayesian calibration of model discrepancy in lower-fidelity models (i.e., piston theory and Eckert's reference temperature method) is used to guide the experimental design. Multiple concurrent measurements are possible, such as aerodynamic pressure, surface temperature, and heat flux. However, the problem is constrained by several practical considerations, including physical limitations on the instrumentation (e.g., clearance of pressure transducers between the panel and wedge, wire bundle size, and maximum operating temperature of sensors), as well as the budget for conducting the test (e.g., specimen fabrication, instrumentation, and wind tunnel run time). The overall objective is to determine the optimal experimental design that will reduce model uncertainty in aerothermoelastic predictions.

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MS78

Semi-supervised Learning using Bayesian Hierarchical Methods

In semi-supervised machine learning, the task of clustering is to divide the data into groups using a labeled subset. Our Bayesian approach to graph-based clustering views the classifying function as a random variable with a distribution that combines the label model with prior beliefs about the classification. In Bayesian hierarchical methods, hyperparameters governing the prior distribution are introduced and can be sampled as well, with the goals of both deriving a classification and learning the distribution of the hyperparameters. We apply dimension-robust hierarchical Markov Chain Monte Carlo methods for indirectly sampling the posterior distribution of these random variables, as direct sampling is generally challenging. We focus on priors derived from the graph Laplacian, a matrix whose eigenvectors are known to contain cluster information. We implemented Bayesian hierarchical models that learn different sets of hyperparameters, including ones that govern the scale of the eigenvectors or the number of eigenvectors used. We tested these models on real and synthetic data sets. Our results indicate that there is information to be learned about the distribution of these hyperparameters, which could be used to improve classification accuracy.

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MS78

Large-data and Zero-noise Limits of Graph-based Semi-supervised Learning Algorithms

Graph-based approaches to semi-supervised classification typically employ a graph Laplacian L constructed from the unlabeled data to provide clustering information. We consider Bayesian approaches wherein the prior is defined in terms of L; choice of data model then leads to probit and Bayesian level set algorithms. We investigate large data limits of these algorithms from both optimization and probabilistic points of view, both when the number of labels is fixed when it grows with the number of data points. We observe a common necessary condition for the limiting algorithms to be meaningful. Finally we consider small noise limits of these algorithms.

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MS78

Robust UQ in Graph-based Bayesian Semi-supervised Learning and Inverse Problems

A popular approach to semi-supervised learning proceeds by endowing the input data with a graph structure in order to extract geometric information and incorporate it into a Bayesian framework. We introduce new theory that gives appropriate scalings of graph parameters that provably lead to a well-defined limiting posterior as the size of the unlabeled data set grows. Furthermore, we show that these consistency results have profound algorithmic implications. When consistency holds, carefully designed graph-based Markov chain Monte Carlo algorithms are proved to have a uniform spectral gap, independent of the number of unlabeled inputs. Several numerical experiments corroborate both the statistical consistency and the algorithmic scalability established by the theory.This is joint work with Zach Kaplan, Thabo Samakhoana and Daniel Sanz-Alonso.

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MS78

Uncertainty Quantification in Graph-based Learning

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MS79

Certified Reduced Basis Method for Nonlocal Diffusion Equations with Application to Uncertainty Quantification

Models of reduced computational complexity is indispensable in scenarios where a large number of numerical solutions to a parametrized problem are desired in a fast/real-time fashion. This is frequently the case for Uncertainty Quantification. Utilizing an offline-online procedure and recognizing that the parameter-induced solution manifolds can be well approximated by finite-dimensional spaces, reduced basis method (RBM) and reduced collocation method (RCM) can improve efficiency by several orders of magnitudes. In this talk, we present our recent development of mathematically rigorous and computationally efficient RBM for nonlocal partial differential equations, with a particular emphasis on nonlocal diffusion equations.

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MS79

Dynamical Low Rank Approximation of Time Dependent Random PDEs

In this talk we consider time dependent PDEs with random parameters and seek for an approximate solution in separable form that can be written at each time instant as a linear combination of linearly independent spatial modes multiplied by linearly independent random variables (low rank approximation) in the spirit of a truncated Karhunen-Love expansion. Since the optimal modes can significantly change over time, we consider here a dynamical approach where those modes are computed on the fly as solutions of suitable evolution equations. We discuss the construction of the method as well as practical numerical aspects for several time dependent PDEs with random parameters, including the heat equation with a random diffusion coefficient; the incompressible Navier-Stokes equations with random Dirichlet boundary conditions; the wave equation with random wave speed. In the latter case, we propose a dynamical low rank approximation that preserves the symplectic structure of the equations.

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MS79

Statistical Modeling of ROM State-space Errors by the ROMES Method

Characterizing the epistemic uncertainty introduced by substituting a full-order model with a reduced-order model (ROM) is crucial for developing rapid yet reliable uncertainty quantification procedures. We present a technique for statistically modeling reduction errors on the solution field (i.e., state) itself arising when a reduced-order model is adopted for the solution of a parametrized partial differential equation (PDE). The proposed technique extends the ROM error surrogate (ROMES) method, which was originally conceived for modeling the error in scalar-valued outputs by using dual-weighted residuals and Gaussian process regression. First, we decompose the state-space error into (i) an in-plane error, and (ii) an out-of-plane error, and represent each of these errors in a unique low-dimensional subspace. Second, we construct an error surrogate for each generalized coordinate characterizing the low-dimensional representation of the in-plane and out-of-plane state-space errors. The resulting error surrogate can then be propagated through any output functional to produce an error surrogate for any scalar or field quantity of interest. Numerical experiments performed on both linear and nonlinear steady PDEs illustrate that the proposed approach improves prediction accuracy of the reduced-order model without incurring significant additional computational costs.

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MS79

Stochastic Sub-modeling under Heterogeneous Input Uncertainty with Application to Coronary Artery Disease

Hemodynamic simulations provide non-invasive assessments of blood flow not obtainable from standard clinical imaging that can aid in disease research. Here we discuss a theoretical/computational approach to simulate hemodynamics under uncertainty from a possibly large number of interacting sources for cases where quantities of interest are referred only to a small portion of the model. Sources from assimilated flow-related inputs are combined with thickness/elastic property parameterizations under the assumption that material property uncertainty does not affect the inference of flow boundary conditions from a lumped peripheral model. We then combine the two uncertainty sources for the analysis of coronary bypass grafts. A reduced order parameterization for coronary bypass submodels is constructed using a sparse orthogonal polynomial representation to map changes in peripheral circulation onto the inlet flow and outlet pressure of the submodel. We also leverage a lower dimensional representation of a random field on a sub model whose size is only a small multiple of an experimentally observed correlation length. We finally perform forward propagation on the reduced model/parameterization with significant computational savings. Results show wall shear stress is associated with limited variance, while material property uncertainty induces significant variability in the wall strain. Results from sensitivity analysis confirm our assumptions on the random inputs.

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MS80

Low-rank Approximations for Efficient MCMC Sampling in Hierarchical Bayesian Inverse Problems

In hierarchical Bayesian inverse problems, the posterior density function depends upon the state vector (often an unknown image) and hyper-parameters. Integrating the posterior density function with respect to the state vector yields the marginal density, defined only over the hyper-parameters. Evaluating the marginal density can be computationally intractable, especially for large-scale and/or nonlinear inverse problems. In this talk, we show how to use low-rank matrices to construct an approximate marginal density that is more computationally efficient to evaluate. We then use this approximate marginal density to develop computationally efficient MCMC methods for sampling from the posterior density functions arising in both linear and nonlinear inverse problems.

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MS80

Methodologies for Enabling Bayesian Calibration in Land-ice Modeling Towards Probabilistic Projections of Sea-level Change

Mass loss from the polar ice sheets is expected to have a significant contribution to future sea-level changes. Predictions of ice sheet evolution are fraught with uncertainty due to unknown model parameters, incomplete knowledge of initial/boundary conditions, uncertain future climate forcing, and sparsity/imprecision of observational data. This talk will describe our ongoing efforts to quantify uncertainties in ice-sheet initial conditions, towards providing uncertainty bounds on expected 21st century sea-level change. First, we will overview our DOE-funded project for land-ice modeling and our land-ice simulation tool, known as ProSPect and FELIX, respectively. Next, we will describe our workflow for estimating in a Bayesian setting the basal friction coefficient, an important high-dimensional parameter that defines the initial/boundary conditions in ice sheet models. This approach is based on a previously-developed computational framework for solving large-scale Bayesian inverse problems (Bui-Thanh et al. 2013; Isaac et al. 2015). The parameter-to-observable map is linearized around the MAP point, computed by solving a large-scale deterministic inversion problem. This leads to a Gaussian posterior distribution whose covariance can be estimated efficiently using a low-rank approximation of the Hessian of the data misfit. Following a discussion of the Bayesian calibration methodology and its implementation, we present results on some realistic Greenland simulations.

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MS80

Randomized Iterative Methods for Bayesian Inverse Problems

In this work, we develop randomized iterative methods to efficiently solve optimization problems that arise in large Bayesian inverse problems. We consider two approaches that exploit randomness to overcome fundamental computational limitations (e.g., data storage and processing, memory allocation, and efficient forward and adjoint model evaluations). One approach follows a randomized stochas-

tic quasi-Newton approach and the other utilizes inexact Krylov methods, where randomization is used to avoid full matrix multiplications. Numerical examples from image processing are provided.

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MS80

Large-p Small-n Nonparametric Regression and Additive-interactive Response Functions

Smoothing based prediction faces many difficulties when the predictor dimension p is large but sample size n is limited, a situation that is often referred to as the large-p small-n prediction problem. A fundamental challenge is that not all smooth functions can be consistently estimated from noisy data if p grows much faster than n. We demonstrate that additive-interactive function spaces offer the ideal modeling framework for consistent estimation. In the additive-interactive model, the mean response function is taken to be the sum total of a modest number of smooth functions each involving a small number of interacting predictors. We show that the minimax L2 estimation rate over such a function space decays to zero under reasonable assumptions on the relative growth rates of n, p and the number of truly active predictors. The additive-interactive assumption naturally leads to a hierarchical Bayesian model for the response function. We introduce a Bayesian estimation method for this model by utilizing an "additive Gaussian process prior" on the model space. We investigate adaptive asymptotic efficiency of this method in prediction under L2 loss and recovery of true predictors.

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MS81

Hamiltonian Monte Carlo-Subset Simulation (HMC-SS) Method for Failure Probabilities and Rare Events Estimation in Non-Gaussian Spaces.

In this talk, we present and promote the use of Hamiltonian Monte Carlo (HMC) method in the context of Subset Simulation (SS) for failure probabilities and rare events estimation. The HMC method uses Hamiltonian mechanics to propose samples following a target probability distribution. Compared to classical Markov-Chain Monte Carlo as Gibbs or Metropolis-Hastings approaches, HMC method alleviates the random walk behavior to achieve a more efficient exploration of the probability space. In this talk, after a brief review of the principles of the HMC method, and subset simulation, we present a series of algorithms to merge the two methods for failure probabilities and rare events estimation. We focus in particular on non-Gaussian spaces, for which the method can be used without transforming the joint probability distribution onto the standard normal space. Finally, we show the accuracy and efficiency of Subset Simulation with the proposed HMC-SS algorithms for a series of benchmark examples.

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MS81

MCMC and Nested Extreme Risks

We design and analyze an algorithm for estimating the mean of a function of a conditional expectation, when the outer expectation is related to a rare-event. The outer expectation is evaluated through the average along the path of an ergodic Markov chain generated by a Markov chain Monte Carlo sampler. The inner conditional expectation is computed as a non-parametric regression, using a least-squares method with a general function basis and a design given by the sampled Markov chain. We establish non asymptotic bounds for the L_2-empirical risks associated to this least-squares regression; this generalizes the error bounds usually obtained in the case of i.i.d. observations. Global error bounds are also derived for the nested expectation problem. Numerical results in the context of financial risk computations illustrate the performance of the algorithms.

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MS81

Ensemble MCMC Samplers for Failure Probability Estimation with Subset Simulation

Subset simulation has, in may respects, become the standard-bearer for estimating failure probabilities - particularly for complex systems with very high dimension. The primary research challenges in subset simulation relate to improving the efficiency and robustness of sampling approaches, specifically Markov Chain Monte Carlo (MCMC) methods. The classical subset simulation algorithm uses a modified Metropolis-Hastings algorithm that decreases the dependence on problem dimension and reduces the number of rejected samples. In the past decade, much work has been performed to improve MCMC algorithms for subset simulation. Recently, a new family of MCMC algorithms referred to as ensemble MCMC samplers have been developed that leverage simultaneously propagating Markov Chains. Ensemble samplers have been shown to reduce sample correlations, dramatically reduce rejection rates especially for degenerate distributions, and reduce the number of parameters necessary for MCMC from a number that scales with the dimension (i.e. typically a length-scale for the proposal density must be specified in every dimension) to only one or two parameters. In this work, we propose a modified form of the affine invariant ensemble MCMC algorithm for applications in subset simulation. This algorithm is particularly effective for estimating failure probabilities in high dimensional systems with lower effective dimension.

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MS81

Bayesian Subset Simulation Tutorial

We consider the problem of estimating a probability of failure α, defined as the volume of the excursion set of a function $f : \mathbb{X} \subseteq \mathbb{R}^d \to \mathbb{R}$ above a given threshold, under a given probability measure on $\mathbb{X}$. In this talk, we present a tutorial about the BSS (Bayesian Subset Simulation) algorithm (Bect, Li and Vazquez, SIAM JUQ 2017), which combines the popular subset simulation algorithm (Au and Beck, Probab. Eng. Mech. 2001) and our sequential Bayesian approach for the estimation of a probability of failure (Bect, Ginsbourger, Li, Picheny and Vazquez, Stat. Comput. 2012). This makes it possible to estimate α when the number of evaluations of f is very limited and α is very small. A key idea is to estimate the probabilities of a sequence of excursion sets of f above intermediate thresholds, using a sequential Monte Carlo (SMC) approach. A Gaussian process prior on f is used to define the sequence of densities targeted by the SMC algorithm, and drive the selection of evaluation points of f to estimate the intermediate probabilities. BSS achieves significant savings in the number of function evaluations with respect to other Monte Carlo approaches. The BSS algorithm is implemented in the STK (Small Matlab/Octave Toolbox for Kriging).

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MS82

Regression Based Methods for Computing Low-rank Tensor-decompositions

Exploiting structure is essential for constructing accurate high-dimensional approximations from limited data. Sparsity and low-rank are two types of structures often present in model response surfaces. In this talk we present regression based methods for constructing low-rank tensor decompositions from unstructured samples. We demonstrate the utility of both linear and non-linear approximation, robust sampling schemes for orthogonal polynomials and discuss connections between low-rank decomposition and sparse approximation.

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MS82

Multilevel Higher-order Quasi-Monte Carlo Bayesian Estimation for PDEs with Random Coefficients

We propose and analyze deterministic multilevel approximations for Bayesian inversion of operator equations with uncertain distributed parameters, subject to additive Gaussian measurement data. The algorithms use a multilevel approach based on deterministic, higher-order quasi-Monte Carlo (HoQMC) quadrature for approximating the high-dimensional expectations, which arise in the Bayesian estimators, and a Petrov-Galerkin (PG) method for approximating the solution to the underlying partial differential equation (PDE). This extends the previous single-level approach from [J. Dick, R. N. Gantner, Q. T. Le Gia and Ch. Schwab, Higher order quasi-Monte Carlo integration for Bayesian estimation, Report 2016-13, Seminar for Applied Mathematics, ETH Zurich (in review)].

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MS82

Multi-scale Sampling Methods for Partial Differential Equations with Gaussian Markov Random Field Inputs

The high computational cost of stochastic simulations involving partial differential equations (PDEs) with uncertain input parameters is often attributable to a combination of two bottlenecks: i) the steep cost of evaluating sample paths and ii) the complexity of the underlying parameter space. In this talk we relate both of these problems to the computational mesh, by using Gaussian Markov random fields to model the PDE's spatially varying input parameters. This allows us to exploit readily available local dependency information of the parameter field in conjunction with sensitivity estimates to identify spatial regions that contribute statistically to the variation in the computed quantity of interest.

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MS82

Estimation of Exciton Diffusion Lengths of Organic Semiconductors in Random Domains

Exciton diffusion length plays a vital role in the function of optoelectronic devices. Oftentimes, the domain occupied by an organic semiconductor is subject to surface measurement error. In this paper, we employ a random function representation for the uncertain surface of the domain. After nondimensionalization, the forward model becomes a diffusion-type equation over the domain whose geometric boundary is subject to small random perturbations. We propose an asymptotic-based method as an approximate forward solver whose accuracy is justified both theoretically and numerically. It only requires solving several deterministic problems over a fixed domain. Therefore, for the same accuracy requirement, we tested here, the running

time of our approach is more than one order of magnitude smaller than that of directly solving the original stochastic boundary-value problem by the stochastic collocation method. In addition, from numerical results, we find that the correlation length of randomness is important to determine whether a 1D reduced model is a good surrogate.

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MS83

Time Discretization Bi-fidelity Modeling

For many practical simulation scenarios, modification of the time-step (large versus small) provides a simple low versus high fidelity scenario in terms of accuracy versus computational cost. Multifidelity approaches attempt to construct a bi-fidelity model having an accuracy comparable with the high-fidelity model and computational cost comparable with the low-fidelity model. In this talk, we present a bi-fidelity framework defined by the time discretization parameter that relies on the low-rank structure of the map between model parameters/uncertain inputs and the solution of interest. We show how this framework behaves on canonical examples, and we show real-world (practical) extensions of our methodology to molecular dynamics simulations.

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MS83

Polynomial Chaos Basis Reduction for Uncertainty Quantification – A Bi-fidelity Approach

Minimization of computational cost is a ubiquitous challenge in uncertainty quantification or design space exploration of fluid mechanics simulations. A useful tool to ease the burden of solving complex systems of PDEs, which arise in such simulations, is model reduction. We present a stochastic basis reduction method in which low-fidelity samples are employed to inform the construction of a reduced basis. Approximating the high-fidelity quantities of interest in this reduced basis requires a small number of high-fidelity samples to achieve a bi-fidelity estimate. The premise of this approach is that while a low-fidelity model may be inaccurate in terms of predicting the quantities of interest, it will represent the stochastic space of the problem for an accurate bi-fidelity approximation. We then present the successful application of this algorithm in two scenarios: a lid-driven cavity and an airfoil. In both cases, we achieve acceptable errors for a minimal number of high-fidelity model evaluations.

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MS83

A Multifidelity Cross-entropy Method for Rare Event Simulation

We introduce a multifidelity approach that leverages a hierarchy of low-cost surrogate models to efficiently construct biasing densities for rare event simulation with importance sampling. Our multifidelity approach is based on the cross-entropy method that derives a biasing density via an optimization problem. We approximate the solution of the optimization problem at each level of the surrogate-model hierarchy, reusing the densities found on the previous levels to precondition the optimization problem on the subsequent levels. With the preconditioning, an accurate approximation of the solution of the optimization problem at each level can be obtained from a few model evaluations only. In particular, at the highest level, only few evaluations of the computationally expensive high-fidelity model are necessary. Our numerical results demonstrate that our multifidelity approach achieves speedups of several orders of magnitude in a thermal and a reacting-flow example compared to the single-fidelity cross-entropy method that uses a single model alone.

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MS84

Multi-level Uncertainty Aggregation with Bayesian Model Error Calibration and Validation

This talk considers the use of data from tests of lower complexity to inform the prediction regarding a complicated system where no test data is available. Typically, simpler test configurations are used to infer the unknown physics model parameters of a system, and the calibration results are propagated through the system model to quan-

tify the uncertainty in the system response. However, the parameter estimation results are affected by the quality of the test configuration model, thus necessitating validation tests of the test configuration model. This talk will present a systematic uncertainty roll-up methodology that integrates calibration and validation results at multiple levels of test configurations towards uncertainty quantification in the system-level prediction. The roll-up methodology also includes a quantitative metric for the relevance of different test configurations to the prediction configuration. A further contribution is the estimation of confidence in using the roll-up distributions of parameters for system-level prediction. An optimization procedure is formulated to maximize the roll-up confidence by selecting the most valuable calibration and validation tests at the lower levels and by designing the selected lower level tests to maximize the information gain. The proposed methods for both the forward and inverse UQ problems are applied to a multi-level dynamics challenge problem developed at Sandia National Laboratories.

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MS84

Calibration and Propagation of Model Discrepancy Across Experiments

Despite continuing advances in statistical inversion and modeling, model inadequacy due to model form error remains a concern in all areas of mathematical modeling. Much like physical models, calibrating a discrepancy model requires careful consideration regarding formulation, parameter estimation, and uncertainty quantification, each of which is often problem-specific. The validity of the original physical model, the inadequacy model, and the combined model for the prediction of quantities of interest remains in question. A generalized approach and implementation of model discrepancy detection, construction, and propagation into a predictive setting is presented in the context of Bayesian model calibration and is demonstrated with an example.

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MS84

Bayesian Model Reduction using Automatic Relevance Determination (ARD): Observations and Improvements

The authors have previously used ARD to perform automatic model reduction for a nonlinear aeroelastic oscillator using Gaussian ARD priors [1]. In this work, we seek to investigate following facets of ARD in the context of Bayesian model reduction: 1) Difference in sparsity levels between LASSO (least absolute shrinkage and selection operator) and ARD, 2) Effect of using different distributions (Uniform, Gaussian, Laplace) for ARD priors on evidence optimization and sparsity levels, 3) Using sequential particle filtering techniques to expedite evidence optimization whereby evidence is computed using an MCMC algorithm.

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MS84

Bayesian Inference of Subsurface Stratification

Abstract not available at time of publication.

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MS85

Multilevel/Multifidelity Monte Carlo for Wave Propagation in Heterogeneous Media

In the last few years efficient algorithms have been proposed for the propagation of uncertainties through numerical codes, however lack of regularity of the solution and high dimensional input spaces still pose a challenge for UQ in realistic configurations. In this scenario Monte Carlo is often the only viable alternative, however its slow convergence rate makes it difficult to apply in the context of expensive high-fidelity simulations. More recently multilevel and multilevel/multifidelity estimators have been introduced in order to increase the reliability of a standard MC estimator by reducing its variance through use of a larger number of coarser/low-fidelity simulations. In this talk we will discuss and apply different multilevel/multifidelity estimators to wave propagation problems in heterogeneous media and we will compare their performance with respect to the standard MC estimator.

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MS85

Efficient Stochastic Galerkin Methods for Uncertainty Quantification of CO2 Storage in Saline Aquifers

Sequestration of CO_2 in subsurface porous media is a key tool for mitigating anthropogenic greenhouse gas emissions causing climate change. In order to ensure safe and secure long time storage it is essential to quantify the influence of parameter uncertainties and reservoir heterogeneity on leakage risk. In this work we apply intrusive uncertainty quantification (UQ) using a Stochastic Galerkin (SG) framework with generalized Polynomial Chaos on a vertically integrated CO_2 transport model. To improve efficiency of the UQ a locally-reduced-order-basis approach and a means for reducing the cost of calculating the SG-matrices is employed. The accuracy and efficiency of the improved SG method is then compared to traditional sampling based UQ.

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MS85

Data-driven Uncertainty Quantification for Transport Problems in Heterogeneous Porous Media

A challenging problem in flow and transport simulations arises in reservoirs that contain channels or other features where the permeability varies discontinuously between channels and surrounding matrix. Traditional two-point statistics methods like Karhunen-Loeve expansions perform poorly in representing these features, but multiple-point statistics methods have been used to successfully to represent channels within a stochastic framework. In this work we use a kernel transformation to create an efficient stochastic parameterization of heterogeneous permeability fields, honoring multiple-point statistics. We then perform forward uncertainty quantification for transport problems using wavelets based on data, combined with stochastic model reduction using analysis of variance (ANOVA) decomposition. The proposed methodology is tested on a problem setup that is representative for reservoirs employed in off-shore CO2 storage in the North Sea.

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MS86

Data-space Inversion for Uncertainty Quantification in Reservoir Simulation and Carbon Storage Applications

Data-space inversion (DSI) enables posterior flow predictions and uncertainty quantification based on prior-model simulation results and observed data. Posterior geological models are not constructed. In previous work, we developed and applied DSI procedures for predicting well-based quantities of interest, such as oil and water production rates. In this talk, new DSI treatments and applications will be presented. First, DSI is extended to enable posterior forecasts, under variable (user-specified) well settings, to be generated without re-simulating any models. This is accomplished by treating new well settings as additional observed data to be matched when posterior DSI predictions are generated. We will demonstrate that this capability facilitates the use of DSI for production optimization under uncertainty. Next, DSI is extended to enable the prediction of CO_2 plume location in carbon storage operations. In this application the data derive from monitoring well observations, and a procedure that efficiently optimizes monitoring well locations is also incorporated. The resulting DSI framework will be shown to provide reasonable predictions for CO_2 plume location, with uncertainty reduced significantly relative to that in prior simulations.

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MS86

A Data-driven Multiscale Finite Volume Method for Uncertainty Quantification

We propose a framework to accelerate multiscale methods within uncertainty quantification by leveraging the repeated computations of basis functions which are obtained by solving localized elliptic problems. Concretely, samples of basis functions are collected from a small number of runs during the uncertainty propagation pipeline. These samples are then used to train a fast regression model of a basis predictor. This predictor then replaces the relatively more expensive computations of localized problems in subsequent forward runs. The effectiveness of the proposed framework is demonstrated on two test cases of multiphase porous media flow.

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MS86

Learning Complex Geologic Patterns for Subsurface Flow Model Calibration

We develop a machine-learning-based framework to aid the reconstruction of complex geological facies maps from limited non-linear measurements in subsurface flow applications. The proposed formulation involves a regularized least-squares problem with a geological feasibility constraint. The least-squares minimization is decomposed into two subproblems that are iteratively solved using the alternating directions algorithm. The first subproblem integrates the nonlinear flow data to obtain approximate continuous solutions, while the second subproblem maps the resulting continuous solution onto a geologically feasible set. The feasible set is defined by prior training models that represent the expected connectivity patterns in the discrete

facies distributions. The mapping of the continuous solution to the feasible set with discrete geologic patterns is implemented using supervised learning via the k-Nearest-Neighbors (kNN) algorithm. Numerical examples are used to evaluate the performance of the method and discuss its important properties.

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MS86

Ultra-fast Reactive Transport Simulations using Machine Learning

Modeling chemical reactions in reactive transport simulations is both challenging and computationally expensive. The involved computations, *chemical equilibrium and kinetics calculations*, can account for over 99% of all computational costs in the simulation. For example, to calculate the chemical equilibrium state of the fluid and solid phases in every mesh cell (or degree of freedom), in every time step, several iterations are needed to solve the underlying non-linear equations governing chemical equilibrium, with each iteration requiring the computation of thermodynamic properties for all species (e.g., activity and fugacity coefficients). In this talk, we present a novel machine learning algorithm that is able to learn on-demand how to perform chemical equilibrium calculations. Whenever the algorithm is applied, it identifies among all previously solved chemical equilibrium problems the one that is closest to the new problem. Once this happens, the machine learning algorithm is able to quickly predict the result, bypassing all those costly operations (evaluation of thermodynamic properties, iterative solution of non-linear equations). If the prediction is not accurate enough, then a *training event* is triggered so that the smart algorithm can learn how to solve similar problems in the future. We show that reactive transport simulations can be performed orders of magnitude faster using the proposed on-demand machine learning algorithm.

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MS87

Variational Reformulation of the Uncertainty Propagation Problem using Probabilistic Numerics

Stochastic partial differential equations (SPDE) have a ubiquitous presence in computational science and engineering. Stochasticity in SPDEs arises from unknown/random boundary/initial conditions or field parameters (e.g., the permeability of the ground in flow through porous media, the thermal conductivity in heat transfer) and, thus, it is inherently high-dimensional. In this regime, traditional uncertainty propagation techniques fail because they attempt to learn the high-dimensional response surfaces (the curse of dimensionality). The only viable alternative is Monte Carlo (and advanced variants such as multi-level MC). However, as A. OHagan put in in his 1987 paper, Monte Carlo is fundamentally unsound because it fails to identify and exploit correlations between the samples. In this work, we develop a promising alternative to MC inspired by recent advances in probabilistic numerics (PN) and variational inference (VI). Our method does not rely on a traditional PDE solver, and it does not attempt to learn a response surface. Instead, we use PN which results in two advantages. First, we gain control over the computational cost, albeit at the expense of additional (but quantified) epistemic uncertainty. Second, PN allows us to quantify the information loss between the true solution of the uncertainty propagation problem and a candidate parameterization. The latter results in a reformulation of the uncertainty propagation problem as a variational inference problem.

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MS87

Uncertainty Quantification for Kinetic Equations

Abstract not available at time of publication.

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MS87

Computational Geometry Aspects of Monte Carlo Approaches to PDE Problems in Biology, Chemistry, and Materials

We will introduce at some Monte Carlo methods for solving problems in electrostatics. These rely on evaluating functionals of the first-passage time of Brownian motion on geometries defined by the system of interest. We will use the Walk on Spheres (WOS) algorithm to quickly evaluate these functionals, and we will show how a computational geometric computation dominates this computation in complexity. We then consider computing the capacitance of a complicated shape, and use this as our model problem to find an efficient serial and parallel implementation. The capacitance computation is prototypical of many Monte Carlo approaches to problems in biology, biochemistry, and materials science. This is joint work with Drs. Walid Keyrouz and Derek Juba from the Information Technology Laboratory at NIST.

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MS87
Distributed Learning

Analyzing and processing big data has been an important and challenging task in various fields of science and technology. Distributed learning provides powerful methods for handling big data and forms an important topic in learning theory.It is based on a divide-and-conquer approach and consists of three steps: first we take a data set stored distributively or divide oversized data into subsets and each data subset is distributed to one individual machine; then each machine processes the distributed data subset to produce one output; finally the outputs from individual machines are combined to generate an output of the distributed learning algorithm. It is expected that a distributed learning algorithm can perform as efficiently as one big machine which could process the whole oversized data, in addition to the advantages of reducing storage and computing costs. This talk describes mathematical analysis of distributed learning.

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MS88
Dakota: Explore and Predict with Confidence

Driven by Sandia National Laboratories' applications, the Dakota project (http://dakota.sandia.gov) invests in both state-of-the-art research and robust, usable software for optimization and UQ. Broadly, Dakota's advanced parametric analysis enables design exploration, model calibration, risk analysis, and quantification of margins and uncertainty with computational models. This presentation will survey challenges with Sandia applications and Dakota capabilities that tackle them. Notably, Dakota has a broad suite of forward and inverse UQ algorithms, including sampling, reliability, stochastic expansions, and non-probabilistic approaches, any of which can be paired with model calibration or design optimization. We will highlight active research and development directions, which include dimension reduction, surrogate modeling, multi-fidelity methods, and inference, together with architecture and usability advances that support their ready use by analysts.

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MS88
The Openturns Uncertainty Quantification Software

OpenTURNS is an open source C++ library for uncertainty propagation by probabilistic methods. Developed in a partnership of four industrial companies (EDF, Airbus, Phimeca and IMACS), it benefits from a strong practical feed-back. Classical algorithms of UQ (central dispersion, probability of exceedance, sensitivity analysis, metamodels) are available and efficientely implemented. Connecting a new simulator to OpenTURNS is easy, thanks to various wrapper services. The OpenTURNS Python module, built on top of the C++ library, is the interface that most users commonly know in practice. However there are situations where we want to perform a UQ study without using a programming language. This is why we developped the graphical user interface (GUI) of OpenTURNS, with the goal of increasing the use of OpenTURNS and, more generally, of the UQ methodology. In this talk, we present the OpenTURNSs GUI within SALOME, an open source platform for pre and post-processing of numerical simulations. Through examples, we discuss the main features of the tool: central dispersion analysis, global sensitivity analysis and threshold probability estimate. We also present advanced graphical features, including the interactive plot matrix view and the parallel coordinate plot available in the GUI and based on the Paraview framework. Finally, we show how the interface can be used within a HPC context, with only a limited input from the user.

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MS88

Data-driven, Adaptive Sparse Grids for UQ in SG++

Adaptive sparse grids provide a flexible and versatile way to represent higher-dimensional dependencies. For UQ, they can be employed to surrogate-based forward propagation as well as for model calibration via density estimation. Therefore, sparse grids have gained increasing interest for UQ. SG++ is the most extensive toolkit for spatially adaptive sparse grids. It is a multi-platform toolkit that excels by fast and efficient algorithms for spatially adaptive sparse grids for UQ and beyond. It provides advanced higher-order basis functions such as B-splines, which can accelerate higher-dimensional stochastic collocation significantly. SG++ supplies operations for sparse grids to compute Jacobian, Hessian matrices, Sobol-indices, or the Rosenblatt transformation for estimated sparse grid densities. SG++ has recently been extended by the sparse grid combination technique (CT / Smolyak rule) that supports a large variety of one-dimensional quadrature rules including new L_2 Leja sequences and global and local polynomial basis functions, and dimensionally adaptive refinement. Transformations are included from CT to spatially adaptive sparse grids and vice versa with proper grid truncation or extension if required. Furthermore, we provide an interface to DAKOTA which makes it possible to obtain a polynomial chaos expansion that is equivalent to the CT solution. We show use cases and its convenient use via its rich interfaces to Python and Matlab.

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MS88

MIT Uncertainty Quantification (MUQ): Bayesian Computation for Statisticaland Physical Problems

MIT Uncertainty Quantification (MUQ) is an open-source software package that provides tools for easily combining models with structure-exploiting uncertainty quantification (UQ) algorithms. MUQ provides a framework for modelers, i.e., experts in their field who are not necessarily versed in the complexities of developing UQ algorithms, to integrate state-of-the-art UQ tools into their workflow. Users decompose both algorithms and physical/statistical models into simple subcomponents, which are connected in a graph that exposes relevant structure. Algorithm subcomponents in MUQ have been designed with a common interface and with attributes that mimic their mathematical formulations, thus simplifying design, facilitating subcomponent exchange, and minimizing the distance between high-level abstractions and code. Users create model subcomponents by writing simple wrappers around existing models; these wrappers define the interface with UQ components and allow MUQ to evaluate the code. Algorithm and model construction is then as simple as defining connections between components. MUQ uses software engineering practices to provide a straightforward graphical structure in a mathematically-aware framework to reduce the effort for domain experts to use UQ algorithms. We have developed state-of-the-art tools for MCMC sampling, constructing sparse polynomial chaos expansions and other surrogate models, modeling random fields, performing inference with transport maps, and more.

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MS89

Targeting a Constrained Traveling Observer by Ensemble Kalman Filter Techniques

We examine the effect of the spatial location of an observation within a Kalman filter data assimilation technique for a nonlinear model of potential meteorological interest. In particular, we model a traveling atmospheric observer subject to a maximum speed constraint, and determine a targeting strategy of this observer based on minimizing the ensemble variance. We then evaluate the performance of this targeting strategy in reducing the forecast error and analysis uncertainty.

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MS89

Targeted Observation Strategy for Space-weather Forecasting During a Geomagnetic Storm

We propose a targeted observation strategy, based on the influence matrix diagnostic, that optimally selects where additional observations may be placed to improve global ionospheric state estimates. This strategy is applied in data assimilation observing system experiments, where a network of synthetic electron density vertical profiles, which represents that of realistic operational satellites, are assimilated into the Thermosphere-Ionosphere-Electrodynamics Global Circulation Model (TIEGCM), using the Local Ensemble Transform Kalman Filter (LETKF), during the 26 September 2011 geomagnetic storm. During each analysis step, the observation vector is augmented with five synthetic vertical profiles optimally placed to target electron density errors, using our targeted observation strategy. Forecast improvement due to assimilation of augmented vertical profiles is measured with the root mean square error (RMSE) of analyzed electron density, averaged over 600 km regions centered around the augmented vertical profile locations. Assimilating vertical profiles with targeted location yields a significant reduction in the RMSE of analyzed electron density and other state variables, such as neutral winds. These results demonstrate that our targeted strategy can improve data assimilation efforts during extreme events by detecting regions where additional observations would provide the largest benefit to the state estimate.

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MS89

Data Assimilation for Irradiance Forecasting

Accurate global horizontal irradiance (GHI) estimates and forecasts are critical when determining the optimal location for a solar power plant, forecasting utility scale solar power production, or forecasting distributed, behind the meter rooftop solar power production. Satellite images provide a basis for producing the GHI estimates needed to undertake these objectives. The focus of this work is to use accurate but sparsely distributed ground sensors to improve satellite derived GHI estimates which cover large areas. We utilize satellite images taken from the GOES-15 geostationary satellite (available every 15-30 minutes) as well as ground data taken from irradiance sensors and rooftop solar arrays (available every 5 minutes). The advection model, driven by wind forecasts from a numerical weather model, simulates cloud motion between measurements. We use the Local Ensemble Transform Kalman Filter (LETKF) to perform the data assimilation. We present preliminary results towards making such a system useful in an operational context. We explain how localization and inflation in the LETKF, perturbations of wind-fields, and random perturbations of the advection model, affect the accuracy of our estimates and forecasts. We present experiments showing the accuracy of our forecasted GHI over forecast-horizons of 15 mins to 1 hr. The limitations of our approach and future improvements are also discussed.

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MS89

Forecast Sensitivity to Observation Impact and Effect of Uncertainty Estimation

In data assimilation that attempts to predict nonlinear evolution of the system by combining complex computational model, observations, and uncertainties associated with them, it is useful to be able to quantify the amount of information provided by an observation or by an observing system. Measures of the observational influence are useful for the understanding of performance of the data assimilation system. The Forecast sensitivity to observation provides practical and useful metric for the assessment of observations. Quite often complex data assimilation systems use a simplified version of the forecast sensitivity formulation based on ensembles. In this talk, we first present the comparison of forecast sensitivity for 4DVar, Hybrid-4DEnVar, and 4DEnKF with or without such simplifications using a highly nonlinear model. We then present the results of ensemble forecast sensitivity to satellite radiance observations for Hybrid-4DEnVart using NOAAs Global Forecast System.

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MS90

Bayesian Computation in Hierarchical Models Using Marginal Local Approximation MCMC

Hierarchical Bayesian models can give rise to inference problems where the actual parameters of interest may be low dimensional relative to the entire state. For instance, one may wish to learn hyperparameters of the prior model in a Bayesian inverse problem, rather than the parameters themselves. Jointly inferring all of the uncertain parameters requires sampling a high dimensional distribution that has complex structure. Moreover, in realistic applications, associated joint density evaluations can be computationally expensive. We address the challenges of sampling and computational cost through a combination of marginalization and surrogate modeling. We construct a Markov chain that directly targets the marginal posterior of the actual parameters of interest. The desired marginal density is often not available analytically; instead, we compute unbiased estimates of this density. We then introduce an MCMC algorithm that progressively synthesizes a *local regression* approximation of the low-dimensional target using these Monte Carlo estimates. Our approach exploits regularity in the marginal density to significantly reduce computational expense relative to both regular and pseudo-marginal MCMC. Continual refinement of the approximation leads to an asymptotically exact characterization of the desired marginal. Analysis of the bias-variance trade-off guides an ideal refinement strategy that balances the decay rates of components of the error.

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MS90

Sampling Hyperparameters in Hierarchical Models

A common Bayesian model is where high-dimensional observed data depends on high-dimensional latent variables that, in turn, depend on relatively few hyperparameters. When the full conditional distribution over latent variables has a known form, general MCMC sampling need only be performed on the low-dimensional marginal posterior distribution over hyperparameters. This gives orders-of-magnitude improvement on popular posterior sampling methods such as random-walk Metropolis-Hastings or Gibbs sampling. For the common linear-Gaussian inverse problem, this marginal-then-conditional decomposition allows the posterior mean to be calculated for *less* compute cost than regularized inversion, as well as providing full uncertainty quantification.

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MS90

Hierarchical Priors in Atmospheric Tomography

Adaptive optics (AO) is a technology in modern ground-based optical telescopes to compensate the wavefront distortions caused by atmospheric turbulence. One method that allows to retrieve information about the atmosphere from telescope data is so-called SLODAR, where the atmospheric turbulence profile is estimated based on correlation data of the wavefront measurements. In this talk we propose a novel extension of the SLODAR concept which corresponds to empirical estimation of a hierarchical prior in a specific inverse problem.

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MS90

Bilevel Parameter Learning in Inverse Imaging Problems

One of the most successful approaches to solve inverse problems in imaging is to cast the problem as a variational model. The key to the success of the variational approach is to define the variational energy such that its minimiser reflects the structural properties of the imaging

problem in terms of regularisation and data consistency. The expressibility of variational models depends on the right choice of parametrisation of regularisation and data consistency terms. Various strategies exist for such a parameter choice, e.g. physical modelling, harmonic analysis, the classical discrepancy principle just to name a few. In this presentation I will discuss bilevel optimisation to learn more expressible variational models. The basic principle is to consider a bilevel optimization problem, where the parametrised variational model appears as the lower-level problem and the higher-level problem is the minimization over the parameters of a loss function that measures the reconstruction error for the solution of the variational model. In this talk we discuss bilevel optimisation, its analysis and numerical treatment, and show applications to regularisation learning, learning of noise models and of sampling patterns in MRI. This talk includes joint work with M. Benning, L. Calatroni, C. Chung, J. C. De Los Reyes, M. Ehrhardt, G. Maierhofer, F. Sherry, and T. Valkonen.

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MS91

Decomposing Functional Model Inputs for Variance-based Sensitivity Analysis

Variance-based sensitivity analysis, developed by Sobol' (1993) and further elaborated by others including Saltelli, Chan and Scott (2000) is a popular technique for assessing the importance of model inputs when there are natural or meaningful probability distributions associated with each input. This approach can be used when some of the model inputs are functions rather than scalar-valued (e.g. Iooss and Ribatet, 2009, and Jacques et al., 2006), but may be somewhat less useful in this case because it does not address the nature of the relationships between functional inputs and model outputs. We consider the option of separating a random function-valued input, represented by a vector of relatively high dimension, into one or a few scalar-valued summaries that are suggested by the context of the modeling exercise, and an independent, high dimensional "residual". We also describe a graphical technique that may help to identify useful low-dimensional function summaries. When the model output is more sensitive to the low dimensional summaries than to the residuals, this is useful information concerning the nature of model sensitivity, and also provides a route to constructing model surrogates with scalar-valued indices that accurately represent most of the variation in the output.

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MS91

Calibration with Frequentist Coverage and Consistency

The resurgence of calibration as a research topic has produced significant work on methods with favorable convergence properties. But there has been a noted lack of conversations about statistically-justified confidence intervals. This talk will give intervals for parameters that, with very few assumptions, contain the underlying best parameter value with the desired confidence, even in small samples. These intervals are also consistent: suboptimal parameters are discarded with probability tending to one.

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MS91

Variable Selection Based on a Bayesian Composite Gaussian Process Model

This talk will describe a variable selection method to identify active inputs to a deterministic simulator code. The methodology is based on a Bayesian composite Gaussian Process (GP) model. This composite model assumes that the output can be described as the sum of a mean plus smooth deviations from the mean. The mean and the deviations are modeled as draws from independent GPs with separable correlation functions subject to appropriate constraints to enforce identifiability of the mean compared with the deviation process. Inputs having smaller estimated correlation parameters are judged to be more active. A reference inactive input is added to the data to judge the size of the correlation parameter for inactive inputs.

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MS91

Calibration for Computer Experiments with Binary Responses

Understanding calibration parameters is often critical when physical and computer experiments are both conducted and there exist unshared input variables. Many methods for experiments with continuous responses have been greatly discussed in literature. On the other hand, with the molecular experiments at hand, calibration method for experiments with binary response is in great demand but has received scant attention. In this paper, we propose an L2 calibration method for computer experiments with binary responses to estimate calibration parameters, and show that the estimators are asymptotically consistent and semiparametric efficient. Numerical examples are examined and show that the method results in accurate estimates. Lastly, we apply the method to molecular experiments; the estimated calibration parameters provide scientific insights in biology which cannot be directly obtainable experimentally.

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MS92

Data-driven Correction of Model and Representation Error in Data Assimilation

Conventional data assimilation assumes that a dynamical model and observation function are both known and correctly specified up to parameterization and noise models. When this assumption fails, the assimilation procedure can produce spurious results and assign them high degrees of confidence. Methods such as adaptive filtering can quantify this model mismatch by comparing filter based forecasts to actual observations and applying statistical tests. In this talk we discuss methods which go beyond quantification of model error and actually correct the model error. By combining reconstructed dynamics from historical data with manifold learning based forecasting and regression methods, we build data-driven auxiliary models which correct the model error in the dynamical and/or observation models. These methods can be used to improve uncertainty quantification for data assimilation and forecasting.

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MS92

Learning Sparse Non-Gaussian Graphical Models from Data

In a Markov network, represented as an undirected probabilistic graphical model, the lack of an edge denotes conditional independence between the corresponding nodes. Sparsity in the graph is of interest as it can, for example, accelerate inference or reveal important couplings within multi-physics systems. Given a dataset from an unknown, continuous, non-Gaussian distribution, our goal is to identify the sparsity of the associated graph. The proposed algorithm relies on exploiting the connection between the sparsity of the graph and the sparsity of transport maps, which deterministically couple one probability measure to another. We present results for datasets drawn from multidisciplinary systems.

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MS92

Bayesian Generative Models for Quantifying Input Uncertainty using Limited Realizations

Quantifying input uncertainty is an essential rather unexplored step before one can proceed with uncertainty propagation. This density estimation problem becomes very challenging when the uncertain input is a random field given in terms of limited realizations. Recently there has been rapid progress in generative models which represent the discretized random field with expressive transforms of simple random variables. These transforms are parameterized using deep neural networks. The expressiveness and advances in training deep learning algorithms enable generative models to approximate the input random field significantly better than other methods. In this work, we extend Generative Adversarial Networks (GANs) to a Bayesian setting to address the challenges of limited realizations and known issues of GANs, such as mode collapse. The improvement and performance of the methodology is illustrated with stochastic reconstruction of heterogeneous random media with applications to geological flows.

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MS92

Bayesian Deep Neural Networks for Surrogate Modeling

We investigate scaling Bayesian inference for deep neural networks with applications to surrogate modeling for computer simulations of stochastic differential equations with high-dimensional input. Approaches to surrogate modeling based on Gaussian processes are attractive because of their Bayesian nature, but are difficult to scale to large data sets. On the other hand, deep neural networks have seen major success in the realm of big data, but Bayesian versions are less developed. In this work, we scale Stein's method for Bayesian neural networks to surrogate modeling appropriate for uncertainty propagation. We illustrate the methodology with standard benchmark problems in the solution of SPDEs as well as other UQ examples where most available techniques fail.

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MS93

Statistical Error Modeling for Approximate Solutions to Parameterized Systems of Nonlinear Equations using Machine Learning

Uncertainty-quantification tasks are often many query in nature, as they require repeated evaluations of a model that often corresponds to a parameterized system of nonlinear equations (e.g., arising from the spatial discretization of a PDE). To make this task tractable for large-scale models, solution approximations (e.g., reduced-order models, coarse-mesh solutions, and unconverged iterations) must be employed. However, such approximations introduce additional error, which may be treated as a source of epistemic uncertainty, that must be quantified to ensure rigor in the ultimate UQ result. We present an approach to

quantify the error (i.e., epistemic uncertainty) introduced by these solution approximations. The approach (1) engineers features that are informative of the error using concepts related to dual-weighted residuals and rigorous error bounds, and (2) applies machine learning regression techniques (e.g., artificial neural networks, random forests, support vector machines) to construct a statistical model of the error from these features. We consider both (signed) errors in quantities of interest, as well as global state-space error norms. We present several examples to demonstrate the effectiveness of the proposed approach compared to more conventional feature and regression choices. In each of the examples, the predicted errors have a coefficient of determination (R^2) value of at least 0.998.

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MS93

Quantifying Unresolved Effects in Reduced Order Models using the Mori-Zwanzig Formalism and Variational Multiscale Method

Quantifying the impact of unresolved scales in unsteady reduced order models is a critical aspect for model prediction and design under uncertainty. This work considers a framework combining the Mori-Zwanzig formalism and Variational Multiscale method (MZ-VMS) as a tool to quantify and model unresolved numerical effects in projection-based reduced order models. The MZ-VMS approach provides a methodology to reformulate a high-dimension Markovian dynamical system as a lower-dimensional, non-Markovian system. In this lower-dimensional system, the impact of unresolved scales on the retained dynamics are embedded in a memory term. This memory term, which is driven by an orthogonal projection of the coarse-scale residual, is used as a starting point to identify and model unresolved dynamics. Examples are presented for unsteady fluid-flow problems.

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MS93

Dimension Reduction of the Input Parameter Space of Vector-valued Functions

Approximation of multivariate functions is a difficult task when the number of input parameters is large. Identifying the directions where the function does not significantly vary is a key step for complexity reduction. Among other dimension reduction techniques, the Active Subspace method uses gradients of a scalar valued function to reduce the parameter space. In this talk, we extend this methodology for vector-valued functions, including multiple scalar-valued functions and functions taking values in functional spaces. Numerical examples reveals the importance of the choice of the metric to measure errors and compare it with the commonly used truncated Karhunen-Loeve decomposition.

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MS93

Efficient PDE-constrained Optimization under Uncertainty using Adaptive Model Reduction and Sparse Grids

This work introduces a framework for accelerating optimization problems governed by partial differential equations with random coefficients by leveraging adaptive sparse grids and model reduction. Adaptive sparse grids perform efficient integration approximation in a high-dimensional stochastic space and reduced-order models reduce the cost of objective-function and gradient queries by decreasing the complexity of primal and adjoint PDE solves. A globally convergent trust-region framework accounts for inexactness in the objective and gradient. The proposed method is demonstrated on 1d and 2d flow control problems and shown to result in over an order of magnitude reduction in computational cost when compared to existing methods.

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MS94

Tuning Asymptotically Biased Samplers with Diffusion Based Stein Operators

As increasingly sophisticated enhanced sampling methods are developed, a challenge that arises is how to tune the simulation parameters appropriately to achieve good sampler performance. This is particularly pertinent for biased sampling methods, which trade off asymptotic exactness for computational speed. While a reduction in variance due to more rapid sampling can outweigh any bias introduced, the inexactness creates new challenges for hyperparameter selection. The natural metric in which to quantify this discrepancy is the Wasserstein or Kantorovich metric. However, the computational difficulties in com- puting this quantity has typically dissuaded practitioners. To address this, we introduce a new computable quality measure using Stein operators constructed from diffusions which quantify the maximum discrepancy between sample and target expectations over a large class of test functions. We will also illustrate applications to hyperparameter selection, convergence rate assessment, and quantifying bias-variance tradeoffs in sampling. This is joint work with Sebastian Vollmer (University of Warwick), Jackson Gorham (Stanford University) and Lester Mackey (Microsoft Research).

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MS94

Irreversible Langevin Samplers, Variance Reduction and MCMC

It is well known in many settings that reversible Langevin diffusions in confining potentials converge to equilibrium exponentially fast. Adding irreversible perturbations to the drift of a Langevin diffusion that maintain the same invariant measure accelerates its convergence to stationarity. When implementing MCMC algorithms using time discretisations of such SDEs, one can append the discretization with the usual Metropolis-Hastings accept-reject step and this is often done in practice because the acceptreject step eliminates bias. However, such a step makes the resulting chain reversible. It is not known whether adding the accept-reject step preserves the faster mixing properties of the non-reversible dynamics. We address this gap between theory and practice by analyzing the optimal scaling of MCMC algorithms constructed from proposal moves that are time-step Euler discretisations of an irreversible SDE, for high dimensional Gaussian target measures. We call the resulting algorithm the ipMALA. To quantify how the cost of the algorithm scales with the dimension N, we prove invariance principles for the appropriately rescaled chain. In contrast to the usual MALA algorithm, we show that there could be two regimes asymptotically: (i) a diffusive regime, as in the MALA algorithm and (ii) a 'fluid' regime where the limit is an ODE. We provide examples where the limit is a diffusion, as in the standard MALA, but with provably higher limiting acceptance probabilities.

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MS94

Noise-robust Metropolis-Hastings Algorithms for Bayesian Inverse Problems

Metropolis-Hastings (MH) algorithms for approximate sampling of target distributions typically suffer from a high dimensional state space or a high concentration of the target measure, respectively. Concerning the first issue dimension-independent MH algorithms have been developed and analyzed in recent years, suitable for Bayesian inference in infinite dimensions. However, the second issue has drawn less attention yet, despite its importance for applications with large or highly informative data. In this talk we consider Bayesian inverse problems with a decreasing observational noise and study the performance of MH algorithms for sampling from the increasingly concentrated posterior measure. In a first analysis we show that employing approximations of the posterior covariance can yield a noise-independent performance of the resulting MH algorithm in terms of the expected acceptance rate and the expected squared jump distance. Numerical experiments confirm the theoretical results and indicate further extensions.

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MS94

Constructing Dimension-independent Particle Filters for High-dimensional Geophysical Problems

Particle filters are approximate solutions to Bayesian Inference Problems. Common wisdom has been that they suffer from the curse of dimensionality, such that they are inefficient in high-dimensional problems. Even the so-called optimal proposal particle filter is proven to need an exponentially growing number of particles with increasing dimension. We will show that this wisdom is based on a misunderstanding of the actual problem, and construct particle filters in which most or all of the particles have equal weight, curing the curse of dimensionality. The basic idea is to generate proposals that to move particles such that they attain a fixed target weight by construction. New filters in this category are derived which minimize the bias present in older versions, providing an important next step in nonlinear high-dimensional Bayesian Inference.

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MS95

Importance Sampling with Stochastic Computer Models

Importance sampling has been used to improve the efficiency of simulations where the simulation output is uniquely determined, given a fixed input. We extend the theory of importance sampling to estimate a system's reliability with stochastic simulations. Thanks to the advance of computing power, stochastic computer models are employed in many applications to represent a complex system behavior. In a stochastic computer model, a simulator generates stochastic outputs at the same input. We develop a new approach that efficiently uses stochastic simulations with unknown output distribution. Specifically, we derive the optimal importance sampling density and allocation procedure that minimize the variance of an estimator. Application to a computationally intensive aeroelastic wind turbine simulation demonstrates the benefits of the proposed approach.

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MS95

Non-Gaussian Models for Extremes

Most physical quantities exhibit random fluctuations which cannot be captured by Gaussian models and non-Gaussian models should be used. Conceptually simple and computationally efficient non-Gaussian models can be divided in two types. The first includes models which match target moments beyond the mean and correlation functions. They are not designed to describe extremes. The second class (translation models) contains memoryless transformations of Gaussian processes. They match target marginal distributions exactly and correlation functions approximately. These models may provide unsatisfactory estimates of extremes since they have independent tails, i.e., the joint distribution of $\big(X_0(s), X_0(t)\big)$ can be approximated by the product of the marginal distributions of the translation

process $X_0(t)$ at times s and t, $s \neq t$, for sufficiently large thresholds. We extend the class of current translation models to processes $X(t)$ defined as memoryless transformations of non-Gaussian processes. These models match exactly target marginal distributions and have dependent tails. Moreover, they can be optimized to characterize accurately quantities of interest e.g. extremes $\max_{0\leq t\leq\tau} \|X(t)\|$ of $X(t)$ over time intervals $[0,\tau]$. We give theoretical arguments and numerical examples to show that one can to construct simple and flexible non-Gaussian images of $X(t)$ and that the proposed translation models provide accurate estimates of extremes.

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MS95

Modified Cross Entropy Based Importance Sampling with a Flexible Mixture Model for Rare Event Estimation

Predicting the probability of a rare event or failure event is of interest in many areas of science and engineering. This probability is defined through a potentially high-dimensional probability integral. Often, the integration domain is only known point-wise in terms of the outcome of a numerical model. In such cases, the probability of failure is usually estimated with Monte Carlo-based sampling approaches, which treat the complex numerical models as a black box input-output relationship. The efficiency of crude Monte Carlo can be improved significantly by importance sampling (IS), provided that an effective IS density is chosen. The cross entropy (CE) method is an adaptive sampling approach that determines the IS density through minimising the Kullback-Leibler divergence between the theoretically optimal IS density and a chosen parametric family of distributions. We present a modified version of the classical CE method that employs a flexible parametric distribution model. We demonstrate the ability of the proposed model to handle low- and high-dimensional problems as well as problems with multimodal failure domains.

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MS95

Adaptive Point Selection for Global vs. Local Surrogate Models

Surrogate models are commonly used to provide a quick approximation of expensive functional evaluations, often for purposes of failure estimation or optimization. The accuracy of surrogates remains an issue for these applications. There are many approaches for adaptively selecting the next best point(s) to add for updating the surrogate after a surrogate is constructed over an initial design. Such adaptive schemes involve metrics such as minimax (space-filling) or choosing the point of maximum prediction variance, with the goal of lowering the overall prediction variance. In this talk, we compare some of the common adaptive sampling schemes for global Gaussian process surrogates with adaptive schemes for local piecewise surrogates based on Voronoi piecewise sampling (VPS). VPS decomposes the parameter space into cells using an implicit Voronoi tessellation around sample points as seeds. It has several advantages over global surrogates in terms of scalability and handling of discontinuous responses. We will present comparisons of accuracy, scalability, and cost of global vs. local adaptive sampling approaches and address batch sampling needs.

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MS96

Analysis of Sparse Approximations in Bayesian Filtering

Bayesian filtering algorithms for systems with nonlinear dynamics and high-dimensional states include ensemble Kalman filters (EnKF), particle filters, and variational Bayesian methods. Given constraints on computational resources, it is common to deploy these algorithms with structured approximations, such as sparse or "localized' covariance or precision matrices in EnKF, or localized weights in certain particle filters. These approximations trade variance for bias, with the goal of preserving stability and improving scalability. In this presentation, we will analyze the tradeoffs resulting from these approximations, focusing on the bias resulting from the imposition of sparse Markov structure (i.e., conditional independence assumptions) or marginal independence assumptions on components of the filtering distribution. We will characterize the associated errors and their evolution in time, and demonstrate our theoretical results in the context of model problems for numerical weather prediction, including stochastic turbulence models and chaotic dynamical systems.

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MS96

Linear Bayesian Inference via Multi-Fidelity Modeling

A significant challenge for Bayesian inference of systems with high-dimensional uncertainty is the calculation of the posterior covariance, as it requires a possibly dense matrix inversion. Recently there have been several works that apply low-rank techniques for posterior covariance approximation to improve upon the associated computational cost. However, in these cases, many high-fidelity model solves are still required, incurring a possibly large computational cost. In this work we consider further cost reduction by introducing the use of a low-fidelity model to form a low-rank, bi-fidelity approximation to the posterior covariance. We will present the formulation of this method as well as

numerical examples demonstrating the achieved cost reduction.

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MS96

Parameter Identification with the Parallel Hierarchical Matrix Technique

We use available measurements to estimate the unknown parameters (variance, smoothness parameter, and covariance length) of a covariance function by maximizing the joint Gaussian log-likelihood function. To overcome cubic complexity in the linear algebra, we approximate the discretized covariance function in the hierarchical (H-) matrix format. The H-matrix format has a log-linear computational cost and storage $\mathcal{O}(kn \log n)$, where the rank k is a small integer and n is the number of locations. The H-matrix technique allows us to work with general covariance matrices in an efficient way, since H-matrices can approximate inhomogeneous covariance functions, with a fairly general mesh that is not necessarily axes-parallel, and neither the covariance matrix itself nor its inverse have to be sparse. We demonstrate our method with Monte Carlo simulations and an application to soil moisture data. The C, C++ codes and data are freely available.

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MS96

Compressed Sparse Tensor Based Approximation for Vibrational Quantum Mechanics Integrals

We propose a method that takes advantage of low rank structure of high dimensional potential energy surfaces in quantum chemistry to find their approximation with very few point evaluations. The low rank approximation is achieved by a synthesis of methods from compressive sensing and low rank canonical tensor decomposition using stochastic gradient descent. This approach is applied on high dimensional integration problems in a quantum chemistry formulation and shows reduction in computation cost by orders of magnitude as compared to the state of the art.

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MS97

Scalable Approximation of PDE-Constrained Optimization under Uncertainty: Application to Turbulent Jet Flow

In this talk, we present a scalable method based on Taylor approximation for PDE-constrained optimal control problems under high-dimensional uncertainty. The computational complexity of the method does not depend on the nominal but only on the intrinsic dimension of the uncertain parameter, thus the curse of dimensionality is broken for intrinsically low-dimensional problems. Further Monte Carlo correction for the Taylor approximation is proposed, which leads to an unbiased evaluation of the statistical moments in the objective function and achieves reduction of variance by several orders of magnitude compared to a Monte Carlo approximation. We apply our method for a turbulence model with infinite-dimensional random viscosity and demonstrate the scalability up to 1 million parameter dimensions.

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MS97

The Role of Variational Multiscale Method in Uncertainty Quantification

The variational multiscale method (VMS) has been extensively used for developing subgrid-scale models that account for the effect of the unresolved scales on the resolved scales in deterministic systems. These models have been used to perform the accurate simulation of such problems on relatively coarse discretizations. In contrast to this, the role of VMS in systems with stochastic parameters has not been fully explored, and is the topic of this talk. In particular, we describe how the VMS method can be used to develop subgrid models for PDEs with stochastic parameters in both intrusive and non-intrusive settings. We also describe how it may be used an an error indicator to drive adaptive discretiztion in the joint physical-stochastic domains.

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MS97

Smoothing Techniques for PDE-Constrained Optimization under Uncertainty

In many areas of the natural sciences and engineering, the underlying phenomena are readily modeled by partial differential equations (PDEs) with random inputs. Once the uncertainty has been propagated through the PDE, the resulting random field PDE solution transforms the usual objective function into a random variable. One possibility to handle this uncertainty in the objective or quantity of interest is to employ risk measures. However, many important risk measures, such as the conditional value-at-risk (CVaR) or mean plus semideviation are non-smooth. The resulting optimization problem is then an often non-convex, non-smooth infinite dimensional problem. Due to the poor performance of off-the-shelf non-smooth solvers for these problems, we propose a variational smoothing technique, which we call epi-regularization. Using epi-regularization, we exploit existing methods for smooth PDE-constrained optimization under unceratinty. The techniques also allows us to prove convergence of minimizers and stationary points. Under local curvature conditions on the reduced objective, we can provide error estimates. We explore the theoretical results by several numerical experiments.

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MS97

Multiscale Optimization and UQ for Additive Manufacturing

Additive manufacturing (AM) is capable of creating compelling designs at a much faster rate than standard methods. However, achieving consistent material properties at various length scales remains a challenge. In this work, we present risk-averse optimization to produce robust designs by tightly controlling certain features of the dynamics while addressing underlying uncertainties. Aspects of the AM process are emulated with PDEs to mimic the behavior of the material during the processing. The goal is to control different aspects of the laser to achieve design targets and simultaneously accommodate uncertainties in different parts of the underlying dynamics. PDE-constrained optimization methods serve as the foundation for this work with finite element discretizations, adjoint-based sensitivities, trust-region methods, and Newton-Krylov solvers. Our final AM produced parts must achieve tight tolerances for a range of different material properties. Accordingly, a range of risk measures are considered with a specific emphasis on reliability. A numerical example coupled to experimental data demonstrates that the use of risk measures as part of the objective function results in optimal solutions and ensures that worse case scenarios are avoided.

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MS98

A Bayesian Framework for Robust Decisions in the Presence of Unobserved Heterogeneity

Measures of decision risk based on the distribution of losses over a posterior distribution obtained via standard Bayesian techniques may not be robust to model misspecification. Standard statistical models assume homogeneity: all individual observables are subject to the same latent variables. Models with covariates relax this assumption by introducing observed sources of heterogeneity. Here we consider model misspecification due to *unobserved sources of heterogeneity* that are not readily captured by known covariates. For example, many predictive physical models contain conservation laws that are globally consistent, but those physical models may be misspecified due to embedded phenomenological models that are only locally consistent within a narrow range of parameters. Instead of fitting a misspecified model to all observations in a data set, we propose fitting the model on multiple subsets of the data where the model has little realized discrepancies—where the homogeneity assumption holds—in order to obtain multiple posterior distributions. By constructing a probability measure over subsets of the data, we can define a *distribution over posterior distributions*, from which we can obtain a distribution of risk measures. This distribution of risk measures allows us to make robust decisions, e.g., by finding an action that minimizes an average expected loss. We will demonstrate these methods on engineering applications of interest.

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MS98

Bayesian Analysis of Boundary Data in EIT: Discrete vs Continuous

Electrical Impedance Tomography (EIT) is an imaging modality in which the goal is to estimate the conductivity distribution inside a body from current/voltage measurements on the boundary of the body. A wealth of mathematical theory on EIT, as well as some direct computational methods, are based on the presumed knowledge of the Dirichlet-to-Neumann map at the boundary, while in reality the data is collected using a fixed set of contact electrodes. In this talk, the mathematical correspondence between the discrete and continuous data is explored, and a computational method of passing from the discrete to continuous data, in the presence of sample-based prior information is described.

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MS98

Use of the Bayesian Approximation Error Approach to Account for Model Discrepancy: The Robin Problem Revisited

We address the problem of accounting for model discrepancy by the use of the Bayesian approximation error (BAE) approach in the context of inverse problems. In many inverse problems when one wishes to infer some primary parameter of interest there are other secondary parameters which are also uncertain. In the standard Bayesian (or deterministic) approach such nuisance parameters are either inverted for or are ignored (perhaps by assignment of some nominal value). However, it is well understood that the ill-posedness of general inverse problems means they do not handle modelling errors well. The BAE approach has been developed as an efficient means to approximately pre-marginalize over nuisance parameters so that one can systematically incorporate the effects of neglecting these secondary parameters at the modelling stage. We motivate the method through an application to the Robin problem governed by the Poisson equation.

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MS98

Analysis of Inadequacy in Simplified Models of Supercapacitor Charge/discharge Cycles

It is common in modeling engineering systems to develop reduced models by starting from a higher fidelity model and introducing simplifying assumptions. In making predictions using the resulting lower fidelity model, it is generally important to represent the effects of these simplifying assumptions (i.e., model inadequacy). Further, the relationship between the high and low fidelity models should be exploited to do so in a manner that is both computationally efficient and physically realistic. In this work, we explore these issues in a simple context: models of supercapacitor charge/discharge cycles. The high fidelity model is PDE based, while the low fidelity model is an ODE based on the PDE behavior in the limit of slow variation of the input current. A stochastic ODE representing the low fidelity model inadequacy is constructed. This model is based upon two realizations about the original low fidelity model. First, the model does not depend correctly on the the time history of the system. Second, the model cannot represent the short time behavior induced by rapid changes in current. The construction of an inadequacy model based on these known deficiencies is discussed, and the performance of the model relative to the high fidelity model is shown.

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MS99

UQ and Parameter Estimation for Coastal Ocean Hazard Modeling

Coastal ocean hazards, including storm surges and tsunamis, affect millions of people worldwide. These hazards may be increasing due to a number of factors, including sea level rise, warming oceans, population growth, and climate variability. In this talk, we will give an overview of coastal hazard modeling, the current state of the art, and needs for the future. We will also discuss many of the uncertainties that are encountered in predictive simulation. We will describe a measure theoretic approach used to calculate uncertain parameters within a stochastic inverse framework. The method will be applied to estimating coastal inundation due to storm surge.

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MS99

Bayesian Inference of Earthquake Parameters for the Chile 2010 Event using Polynomial Chaos-based Surrogate and Buoy Data

We are interested in the Bayesian inference of earthquake parameters associated with the Chile 2010 event. The goal is to infer the location, orientation as well as the slip parameter of an Okada model of the fault from real data collected at a single DART station. Several challenges are addressed in this work concerning the development of a statistical model, a surrogate model and its goal-oriented reduction that are robust concerning the limitations of the numerical model and the data. First, a non-stationary correlated Gaussian noise is introduced to model the discrepancy between the data and the numerical model. The posterior distribution is then sampled using an adaptive Metropolis-Hastings algorithm. A surrogate model is constructed to accelerate the inference using two polynomial chaos expansions computed by non-intrusive spectral projection. We

first approximate the arrival time of the waves at the station and define a fictitious time such that, for every parameter value, the wave reaches the gauge at a prescribed instant. In this fictitious time, the water elevation with respect to the parameter is regularized, and a polynomial chaos expansion can be used. Finally, a singular value decomposition based on the Mahalanobis distance is introduced to reduce the model while preserving the posterior distribution of the inferred parameter. Numerical results are presented and discussed.

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MS99

Earthquake Source Dimension Reduction with Gaussian Process Emulation: Quantification of Tsunami Hazard

Tsunami hazard assessment requires the propagation of tsunami source uncertainties to the distributions of relevant quantities in the affected areas. The physics is captured by a coupled two-stage deterministic model; the tsunamigenic seabed deformation caused by the earthquake source, and subsequent propagation of the tsunami to affected coasts. The corresponding numerical codes are computationally expensive. We overcome this by building statistical surrogates (or emulators) of the models that provide faster and cheaper approximations. These Gaussian process emulators are then used to propagate the uncertainties in the source to the wave heights at the coasts. The uncertainties in the source (slips) are modeled using a geo-statistical approach whilst encapsulating regional geophysical knowledge. The high dimensionality of the source presents a significant hurdle in the emulator construction. Thus, we merge the emulator construction with a gradient-based kernel dimension reduction to decrease dimensionality while also reducing the loss in information. We illustrate the framework using the case of the potential tsunamigenic zone in the Makran region.

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MS99

Probabilistic Tsunami Hazard Assessments with Consideration of Uncertain Earthquake Characteristics

The uncertainty quantification of tsunami assessments due to uncertain earthquakes faces important challenges. First, the generated earthquake samples must be consistent with past events. Second, it must adopt an uncertainty propagation method to determine tsunami uncertainties with a low computational cost. In this study we propose a new methodology, which improves the existing tsunami uncertainty assessment methods. The methodology considers two uncertain earthquake characteristics, the slip and location. First, the methodology considers the generation of consistent earthquake slip samples by means of a Karhunen Loeve expansion and a translation model, applicable to any non-rectangular rupture and marginal distribution. Furthermore, we preserve the original probability properties of the slip distribution by avoiding post sampling treatments, such as earthquake slip scaling. Second, the methodology uses the stochastic reduced order model SROM (Grigoriu, 2009) instead of a Monte Carlo simulation, which reduces the computational cost of the uncertainty propagation. The methodology is applied on real study cases. We demonstrate that our stochastic approach generates consistent earthquake samples with respect to the target probability laws. We also show that the results obtained from SROM are more accurate than classic Monte Carlo simulations.

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MS100

Identification of Primary Flow Regions Through Three-dimensional Discrete Fracture Networks using Supervised Classification and Graph-based Representations

Discrete fracture network (DFN) models are designed to simulate flow and transport in fractured porous media. Flow and transport calculations reveal that a small backbone of fractures exists, where most flow and transport occurs. Restricting the flowing fracture network to this backbone provides a significant reduction in the network's effective size. However, the particle tracking simulations needed to determine the reduction are computationally intensive. Such methods are impractical for large systems or for robust uncertainty quantification of fracture networks, where thousands of forward simulations are needed to bound system behavior. We present a graph-based method to identify primary flow and transport subnetworks in three-dimensional fracture networks. Coupled with supervised machine learning techniques the method efficiently identifies these backbones while also revealing key characteristics of flow and transport through fractured media.

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MS100

Deep Residual Recurrent Neural Network for Model Reduction

Recently, proper orthogonal decomposition (POD) combined with Galerkin projection has been applied more frequently to overcome the computational burden of multiquery tasks (e.g. uncertainty quantification, model based optimization) governed by large scale nonlinear partial differential equations (PDEs). However, the effectiveness of POD-Galerkin based reduced order model (ROM) in handling nonlinear PDEs is limited mainly by two factors. The first factor is related to the treatment of the nonlinear terms in the POD-Galerkin ROM and the second factor is related to maintaining the overall stability of the resulting ROM. In this talk, we combine deep residual recurrent neural network (DR-RNN) with POD-Galerkin and discrete empirical interpolation method (DEIM). DR-RNN is a physics aware recurrent neural network for modeling the evolution of dynamical systems. The DR-RNN architecture is inspired by iterative update techniques of line search methods where a fixed number of layers are stacked together to minimize the residual of the physical model under consideration. We demonstrate the accuracy and stability property of DR-RNN on two forward uncertainty quantification problems involving two-phase flow in subsurface porous media. We show that DR-RNN provides accurate and stable approximations of the full-order model in comparison to standard POD-Galerkin ROMs.

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MS100

Deep Learning and Dynamic Mode Decomposition for Modeling the Dynamics of Oil & Gas Problems

In this work, we introduce and investigate the performance of Convolutional and Recurrent Neural Networks (CNNs and RNNs) and the recently proposed Dynamic Mode Decomposition (DMD) for modeling complex dynamical systems. The application of any of the aforementioned methods is basically new as viable alternatives to produce data-driven models capable of capturing the dynamics of complex and different Oil & Gas problems. CNN and RNN represent two of the most successful Deep Learning (DL) architectures for generating accurate predictions from image and time series data representations, respectively. However, DL methodologies are still unclear alternatives to produce business value propositions in the Oil & Gas industry. On the other hand, DMD appears as a data-driven model reduction approach that assumes that complex patterns can be decomposed into a simple representation based on spatiotemporal coherent structures amenable to produce future states and observable responses. Analysis of DL and DMD and their comparison provides elements for enhancing capabilities not only for prediction but also for optimization and control of complex dynamical systems. By bringing up a few use cases, we show that both DL and DMD approaches have the potential to provide faster and reliable alternatives to overcome the high computational cost entailed by multiple processes in the industry.

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MS101

A Robust Stochastic Galerkin Method for the Compressible Euler Equations with Uncertainty

It is known that the stochastic Galerkin method applied to hyperbolic systems such as the compressible Euler equations subject to random inputs may lead to an enlarged system which is not necessarily hyperbolic. In addition, such a method usually relies on the positivity of some macroscopic quantities (e.g. sound speed), which may break down when solution presents severe discontinuities. We introduce a stochastic Galerkin method for the compressible Euler equations based on a kinetic formulation. The method solves the Boltzmann equation efficiently for a large range of Knudsen numbers and reduces to an approximated (regularized) solver for the Euler equations when the Knudsen number is small. Furthermore, the method does not need to evaluate any macroscopic quantities nor require their values to be positive, hence is especially suited for problems involving discontinuities. Joint work with Shi Jin and Ruiwen Shu.

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MS101

Analysis and Application of Stochastic Collocation Method for Maxwells Equations with Random Coefficients

In this talk, we will present the development and analysis of the stochastic collocation method for solving the time-dependent Maxwell's equations with random coefficients and subject to random initial conditions. We provide a rigorous regularity analysis of the solution with respect to the random variable. To our best knowledge, this is the first theoretical results derived for the stochastic Maxwell's equations. The rate of convergence is proved depending on the regularity of the solution. Numerical results are presented to confirm the theoretical analysis. Extensions of this analysis and applications to Maxwell's equations in random Drude metamaterials will be discussed too.

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MS101

Inferring the Biological Networks via Information

Theoretic Approaches

Partial correlation (PC) or conditional mutual information (CMI) is widely used in detecting direct dependencies between the observed variables in a network by eliminating indirect correlations/associations, but it fails whenever there are some strong correlations in the network, due to the inherent underestimation problem of PC/CMI. We theoretically develop a multiscale association analysis to overcome this difficulty. Specifically, we first show why conditional mutual information (CMI)/partial correlation (PC) suffers from an underestimation problem for biological networks with strong correlations. Then, we propose a new measure, partial association (PA), based on the multiscale conditional mutual information (MCMI), to solve this problem. We show that linear PA and nonlinear PA can quantify the direct associations in biological networks in an accurate manner from both theoretical and computational aspects. Both simulated models and real datasets demonstrate that PA is superior to PC and CMI in terms of efficiency and effectiveness, and is a powerful tool to identify the direct associations or reconstruct the biological network based on the observed omics data.

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MS101

Stochastic Methods for the Design of Random Meta-materials under Geometric Constraints

Nanostructured materials such as a meta-surface for solar cell applications provide new opportunities for efficient light trapping. We present a computational stochastic methodology to generate random configurations of meta-materials with optimized properties. The main components of the methodology are: (1) A deterministic solver for electromagnetic scattering from multiple objects. (2) The Karhunen-Loeve expansion to represent the correlated configurations of the scattering objects. (3) The Multi-element probabilistic collocation method (MEPCM) to have flexibility in adopting different probability distributions for the configurations. MEPCM is used in combination with the adaptive ANOVA decomposition and sparse grids to investigate the sensitivity of the transmission and reflection coefficients to different parameters and deal with dimensionality challenges. To characterize the randomness of the configurations we employ random fields (RFs) from a Spartan family that includes covariance functions with a damped oscillatory behavior. We study light propagation through randomly spaced heterojunctions and multi-dimensional structures. We found that greater transmission and reflection, compared to the uniformly spaced structures, can be achieved for a structure with an oscillatory spacing profile. Optimized configurations for different wave numbers and angles of the incoming wave, as well as different parameters of the RFs, are found.

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MS102

URANIE: The Uncertainty and Optimization Platform

URANIE developed by CEA is a framework to deal with uncertainty propagation, sensitivity analysis, surrogate models, code calibration and design optimization. URANIE is a free and Open Source multi-platform (Linux and Windows) based on the data analysis framework ROOT, an object-oriented and petaflopic computing system developed by the CERN. This framework provides all the functionalities needed to deal with big data processing, statistical analysis, visualisation and storage. It is mainly written in C++ but integrated with other languages such as Python and R.

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MS102

Mystic: Rigorous Model Certification and Engineering Design under Uncertainty

Highly-constrained, large-dimensional, and nonlinear optimizations are at the root of many difficult problems in uncertainty quantification (UQ), risk, operations research, and other predictive sciences. The 'mystic' software was built to solve large non-convex optimization problems, with nonlinear constraints. Mystic leverages parallel computing to provide fast global optimization, interpolation, and surrogate construction over difficult nonlinear surfaces, and additionally provides a general mechanism for the direct application of constraining information as reductions to optimizer search space. With these tools, mystic enables the solving of difficult UQ and engineering design problems as global optimizations.

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MS102

Cossan Software: Recent Advancements and Case Studies

Cossan is a general purpose software package to quantify, mitigate and manage risk and uncertainty. The package offers the most advanced and recent algorithms for Simulation-based Reliability Analysis, Sensitivity Analysis, Meta-Modelling, Stochastic Finite Elements Analysis

(SFEM), and Reliability-Based Optimization (RBO). Including full interaction with any third-party solvers, and combination of available algorithms with specific solution sequences, Cossan provides the framework to tackle the challenges of both academia and industry. We will provide updates on the most recent additions to the Cossan libraries with some examples. Robust Artificial Neural Network library, to improve the prediction robustness of an ANN based on coupling Bayesian framework and model averaging techniques. Interval Predictor Models (IPMs) toolbox, IPMs are a class of meta-model which describe the expected spread of the output of a model whilst making very few assumptions about the model. The Credal Network Toolbox, for Bayesian Belief Network construction, a probabilistic graphical model based on the use of directed acyclic graphs, integrating graph theory with the robustness of Bayesian statistics. Finally the System Reliability Toolbox, allowing users to construct multi-component systems within the Cossan environment, and investigate the behaviour of such systems. http://www.cossan.co.uk.

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MS102

Foqus-PSUADE: A Framework for Uncertainty Quantification and Optimization

PSUADE (Problem Solving environment for Uncertainty Analysis and Design Exploration) is a general-purpose software tool for non-intrusive ('black box' simulation models) uncertainty quantification. This talk will begin with a brief overview of PSUADE's core capabilities, followed by a discussion of recent enhancements as well as future development efforts. Practical development issues such as user interface development will also be addressed.

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MS103

Long Term Integration of Burgers Equation with Rough Noise

We propose a restarted stochastic collocation methods for Burgers equation driven by white noise. The standard stochastic collocation methods suffer from the curse of dimensionality. To reduce the dimensionality in random space, we apply independent component analysis to reconstruct the computed solutions every few time steps. After such a reconstruction, we then march in time and compute solutions with appropriate stochastic collocation methods and repeat the aforementioned procedure until desired integration time instant. Numerical results and some basic analysis of the proposed methodology will be presented.

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MS103

Mixed Finite Element Methods for the Stochastic Cahn-Hilliard Equation with Gradient-type Multiplicative Noises

In this talk, we will study finite element approximations for the stochastic Cahn-Hilliard equation with gradient-type multiplicative noise that is white in time and correlated in space. The sharp interface limit as the diffuse interface thickness vanishes of the stochastic equation formally approximates a stochastic Hele Shaw flow which is described by a stochastically perturbed geometric law of the deterministic Hele Shaw flow. Both the stochastic Cahn-Hilliard equation and the stochastic Hele Shaw flow arise from materials science, fluid mechanics and cell biology applications. Two fully discrete finite element methods which are based on different time-stepping strategies for the nonlinear term are proposed. Strong convergence with sharp rates for both fully discrete finite element methods is proved. This is done with the crucial help of the Hölder continuity in time with respect to the spatial L^2-norm and H^1-semi-norm for the strong solution of the stochastic Cahn-Hilliard equation, which are key technical lemmas. It is proven that the error estimates hold on a set which is close enough to the whole domain. Numerical experiments are provided to gauge the performance of the proposed fully discrete finite element methods and to study the interplay of the geometric evolution and gradient-type noise.

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MS103

Reduced Order Models for Uncertainty Quantification of Time-dependent Problems

In many time-dependent problems of practical interest the initial conditions needed can exhibit uncertainty. One way to address the problem of how this uncertainty impacts the solution is to expand the solution using polynomial chaos expansions and obtain a system of differential equations for the evolution of the expansion coefficients. We present an application of the Mori-Zwanzig formalism to the problem of constructing reduced models of such systems of differential equations. In particular, we construct reduced models for a subset of the polynomial chaos expansion coefficients that are needed for a full description of the uncertainty. We show with several examples what are the computational issues arising from the application of the formalism and how they can be addressed.

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MS104

Replication or Exploration? Sequential Design for Stochastic Simulation Experiments

We investigate the merits of replication, and provide methods that search for optimal designs (including replicates), in the context of noisy computer simulation experiments. We first show that replication offers the potential to be beneficial from both design and computational perspectives, in the context of Gaussian process surrogate modeling. We then develop a lookahead based sequential design scheme that can determine if a new run should be at an existing input location (i.e., replicate) or at a new one (explore). When paired with a newly developed heteroskedastic Gaussian process model, our dynamic design scheme facilitates learning of signal and noise relationships which can vary throughout the input space. We show that it does so efficiently, on both computational and statistical grounds. In addition to illustrative synthetic examples, we demonstrate performance on two challenging real-data simulation experiments, from inventory management and epidemiology.

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MS104

Interleaved Lattice-based Minimax Distance Designs

We propose a new method for constructing minimax distance designs, which are useful for computer experiments. To circumvent computational difficulties, we consider designs with an interleaved lattice structure, a newly defined class of lattice that has repeated or alternated layers based on any single dimension. Such designs have boundary adaptation and low-thickness properties. From our numerical results, the proposed designs are by far the best minimax distance designs for moderate or large samples.

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MS104

Leverage Values of Gaussian Process Regression and Sequential Sampling

In this work, we define the hat matrix and the leverage values for the Gaussian Process regression models. We discover some interesting properties of them that resemble the hat matrix and leverage values of the linear regression model. We also generalize the original definition of Cook Distance to GP regression that can be used to search for outliers. The second part of the paper develop the sequential sampling procedure based on the leverage, and we compared it with other alternatives. Examples on simulation and real data are illustrated to show the performances of the proposed methods.

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MS104

Robust Designs for Gaussian Process Modeling of Computer Experiments

We introduce in this presentation two new classes of experimental designs, called support points and projected support points, which can provide robust and effective emulation of computer experiments under Gaussian process modeling. These designs have three important properties which are appealing for modeling computer experiments. First, the proposed designs are robust, in that they enjoy excellent emulation performance over a wide class of smooth and rugged response surfaces. Second, these designs can be shown to address several shortcomings in existing computer experiment designs, both in theory and in practice. Lastly, both support points and projected support points can be efficiently generated for large designs in high dimensions. In this presentation, we first present a theoretical framework illustrating the above properties, then demonstrate the effectiveness of the proposed designs over state-of-the-art methods in simulations and real-world computer experiments.

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MS105

Optimal Information Acquisition Algorithms for Inferring the Order of Sensitivity Indices

Numerous engineering problems are characterized by expensive simulation/experiment as objective functions, where the goal is to identify regions of design space which satisfy a set of criteria defined at the outset (which includes optimization cases). In many engineering applications, it is of key interest to understand which design variables drive changes in the objectives and to compute the relative order of importance. This question is answered via a combination of data-driven modeling and global sensitivity analysis where so-called sensitivity indices are computed. Towards this, Bayesian global sensitivity analysis (BGSA) constructs a computationally cheap probabilistic surrogate of the expensive objective function(s) using Gaussian Process (GP) regression. The surrogate provides approximate samples of the underlying function. We propose an algorithm that evaluates the merit of a hypothetical measurement towards the segregation of the individual sensitivity indices. This framework guides the designer towards evaluating the objective function to acquire information about the sensitivities sequentially. We verify and validate the proposed methodology by applying it on synthetic test problems. We then demonstrate our approach on a real-world industry engineering problem of optimizing a compressor for oil applications. The problem is characterized by an expensive objective (lab tests; each taking 1-2 days) and a high-dimensional input space with 30 input variables.

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MS105

A Spectral Approach for the Design of Experiments: Design, Analysis and Algorithms

This talk discusses a new approach to construct high quality space-filling sample designs. First, we propose a novel technique to quantify the space-filling property and optimally trade-off uniformity and randomness in sample designs in arbitrary dimensions. Second, we connect the proposed metric (defined in the spatial domain) to the objective measure of the design performance (defined in the spectral domain). This connection serves as an analytic framework for evaluating the qualitative properties of space-filling designs in general. Using the theoretical insights provided by this spatial-spectral analysis, we derive the notion of optimal space-filling designs, which we refer to as space-filling spectral designs. Third, we propose an efficient estimator to evaluate the space-filling properties of sample designs in arbitrary dimensions and use it to develop an optimization framework to generate high quality space-filling designs. Finally, we carry out a detailed performance comparison on two different applications in 2 to 6 dimensions: a) image reconstruction and b) surrogate modeling on several benchmark optimization functions and an inertial confinement fusion (ICF) simulation code. We demonstrate that the propose spectral designs significantly outperform existing approaches especially in high dimensions.

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MS105

Stochastic Dimension Reduction using Basis Adaptation and Spatial Domain Decomposition for PDEs with Random Coefficients

In this work, we present a stochastic dimension reduction method based on the basis adaptation in combination with the spatial domain decomposition method for partial differential equations (PDEs) with random coefficients. We use polynomial chaos based uncertainty quantification (UQ) methods to solve stochastic PDEs and model random coefficient using Hermite polynomials in Gaussian random variables. In this approach, we decompose the spatial domain into a set of non-overlapping subdomains, and find in each subdomain a low-dimensional stochastic basis to represent the local solution in that subdomain accurately. The local basis in each subdomain is obtained by an appropriate linear transformation of the original set of Gaussian random variables spanning the Gaussian Hilbert space. The local solution in each subdomain is solved independently of each other while the continuity conditions for the solution and flux across the interface of the subdomains is maintained. We employ Neumann-Neumann algorithm to systematically compute the solution in the interior and at the interface of the subdomains. To impose continuity, we project local solution in each subdomain onto a common basis. We show with the numerical experiments that the proposed approach significantly reduces the computational cost of the stochastic solution.

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MS106

Padé Approximation for Helmholtz Frequency Response Problems with Stochastic Wavenumber

Due to the oscillatory behavior of the analytic solutions, the finite element approximation of the Helmholtz boundary value problem in mid- and high-frequency regimes is computational expensive and time-consuming: accurate approximations are possible only on very fine meshes or with high polynomial approximation degrees. For this reason, when solutions at many frequencies are of interest, repeated finite element computations become prohibitive. To reduce the computational cost we propose a model order reduction method based on Least Square Padé-type techniques. In particular, the Helmholtz frequency response map - which associates each frequency with the corresponding solution of the Helmholtz boundary value problem - is approximated starting only from precomputed evaluations at few frequency values. Uniform convergence results of the Least Square Pad approximation error are proved. Two algorithms to compute the Least Square Pad approximant are discussed. 2D numerical tests are provided that confirm the theoretical upper bound on the convergence error. This is joint work with Fabio Nobile and Davide Pradovera (EPFL), and Ilaria Perugia (University of Vienna).

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MS106

Reduced Order Models for CVaR Estimation and Risk Averse Optimization

Two reduced order model (ROM) approaches for CVaR estimation are introduced and analyzed. One replaces the original quantity of interest by the ROM approximation. The other uses ROMs to generate importance sampling. Improvements gained by using ROMs are quantified and illustrated numerically. These CVaR estimation approaches are then used to optimize CVAR subject to PDE constraints with uncertain parameters. In this context it is important that key quantities that need to be approximated for CVAR objective function evaluations are also the key quantities arising in gradient computations. Nu-

merical results are given to illustrate the performance gains due to ROM. This talk is based on joint work with Boris Kramer (MIT), Timur Takhtaganov (Rice), and Karen Willcox (MIT).

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MS106

Multifidelity Dimension Reduction via Active Subspaces

Engineering problems such as optimization and inference become increasingly challenging as the dimension of the problem grows. In some cases, most of the variations of the function of interest can be captured by a low-dimensional subspace. Identifying and exploiting this subspace reduces the complexity of solving the problem at hand. The active subspace method leverages gradient information to compute such subspace. In this work, we propose to use multifidelity techniques to reduce the cost of identifying the active subspace. We provide an analysis of the number of gradient evaluations necessary to achieve a prescribed error in expectation and with high probability. Numerical experiments illustrate the benefits of such an approach.

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MS106

Low-rank Methods for Approximations of Posterior Covariance Matrix of Linear Bayesian Inverse Problems

We consider the problem of efficient computations of the covariance matrix of the posterior probability density for linear Gaussian Bayesian inverse problems. However, the covariance matrix of the posterior probability density is dense and large. Hence, the computation of such a matrix is impossible for large dimensional parameter spaces as is the case for discretized PDEs. Low-rank approximations to the posterior covariance matrix were recently introduced as promising tools. Nevertheless, the resulting approximations suffer from the curse of dimensionality for transient problems. We here exploit the structure of the discretized PDEs in such a way that spatial and temporal components can be separated and the curse overcomes. We reduce both the computational complexity and storage requirement from $\mathcal{O}(n_x n_t)$ to $\mathcal{O}(n_x + n_t)$[1] Here n_x is the dimension of the spatial domain and n_t is the dimension of the time domain. We use numerical experiments to illustrate the advantages of our approach. [1] P. Benner, Y. Qiu, and M. Stoll. Low-rank computation of posterior covariance matrices in Bayesian inverse problems, *arXiv:1703.05638*, 2017.

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MS107

Bayesian Algorithms for Data-driven Turbulence Modelling

Recently several researchers have started to use Bayesian methods in the context of turbulence modelling - to obtain an empirical map from feature space consisting of the local mean-flow, to the Reynolds-stress tensor (RST), using reference data (LES, DNS) to train the model. However, no such unique map exists, and current techniques to not take into account the scatter in possible RSTs for a given feature vector. We aim to construct a stochastic map based on a generalised Gaussian process, fitted to the mean, variance, and (local) correlation-length of the reference data in feature-space. Realizability and Galilean invariance of the RST are naturally enforced. Random samples generated from our map are propagated through a solver with MC and MLMC to predict flows not in the training-set. The quantified uncertainty of these predictions is compared with held-back reference data.

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MS107

Uncertainty Propagation in RANS Simulations via Multi-level Monte Carlo Method

A Multilevel Monte Carlo (MLMC) method for quantifying model-form uncertainties associated with the Reynolds-Averaged Navier-Stokes (RANS) simulations is presented. Two high-dimensional local stochastic extensions of the RANS equation are considered to demonstrate the applicability of MLMC method. The first approach is based on global perturbation of the baseline eddy-viscosity field using a log-Gaussian random field. A more general second extension is also considered where the entire Reynolds Stress Tensor (RST) is perturbed while maintaining realizability. Two fundamental flow problems are studied, showing the practical advantage of the multilevel Monte Carlo method over the standard Monte Carlo methods.

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MS107

Constitutive Modeling of Turbulence with Physics-informed Machine Learning

Reynolds-averaged Navier-Stokes (RANS) models are

widely used in simulating turbulent flows in engineering applications. The modeling of Reynolds stress introduces large model-form uncertainties, diminishing the reliability of RANS simulation results. In this talk, we present a data-driven constitutive modeling approach by using physics-informed machine learning. This framework consists of three components: (1) build a neural-network-based constitutive model for turbulence, (2) impose physical constraints to that neural-network-based constitutive model, and (3) use the machine-learning-trained constitutive model to simulate mean velocity field and other quantities of interest. We evaluate the performance of proposed data-driven constitutive modeling approach by using the flows with stress-induced secondary flow and flows with massive separation, both of which are challenging for traditional RANS modeling. Significant improvements over the baseline RANS simulation are observed.

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MS107

Bayesian Modeling of Mixed Aleatory and Epistemic Uncertainty in CFD

The problem of mixed aleatory/epistemic uncertainty quantification applied to computationally expensive models is considered. Aleatory uncertainty is irreducible uncertainty which is often characterized by probability density functions. Epistemic uncertainty is introduced by lack-of-knowledge and errors in the models under consideration and can be reduced by investing more effort in modeling (e.g. by investing more computational time or using more accurate models). Our approach to model these uncertainties is fully Bayesian. The unknown epistemic uncertainty is characterized using the concept known as Bayesian model calibration. The aleatory uncertainties are combined with the resulting posterior such that predictions under uncertainty can be made efficiently. The novelty of our approach is a new sampling procedure, requiring significant less samples than conventional methods to produce accurate results. We propose an adaptive methodology that replaces the (computational expensive) model with an interpolating surrogate that is based on weighted Leja nodes.

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MS108

Rare Event Probability Estimation using Adaptive Support Vector Regression - Importance of Kernels and their Proper Tuning

The presentation is about surrogate models used for the estimation of rare event probabilities. In this context support vector regressors (SVR) are adaptively constructed as surrogates of expensive-to-evaluate functions. The following important aspects are addressed in the talk: choice of kernel type (e.g. isotropic vs. anisotropic), tuning of SVR hyperparameters, selection criteria for enriching the training set of data. The efficiency and robustness of the proposed adaptive method are assessed from a set of challenging examples with a comparison to published results obtained by other methods where available.

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MS108

Sequential Designs of Surrogate Models for Reliability Analysis

Reliability analysis estimates the probability of a rare event, the failure event. Efficient estimation of the probability of failure can be performed with sequential importance sampling methods. These methods sample a sequence of measures that gradually approach the theoretically optimal importance sampling density. To facilitate efficient estimation for cases where the failure event is defined in terms of the outcome of a computationally intensive numerical model, sequential importance sampling approaches can be combined with surrogate models. We consider the construction of multiple low-fidelity surrogate models through building polynomial chaos expansions (PCEs) at each intermediate measure/sample set provided by the sequential sampling procedure. By design, these surrogates will be most accurate on the support of the current intermediate measure/sample set. To address the curse of dimensionality, we consider the construction of order-reduced PCEs in rotated spaces as suggested in [R. Tipireddy, R.G. Ghanem, Basis adaptation in homogeneous chaos spaces, J. Comput. Phys. 259 (2014) 304317] after eliciting important directions pointing towards the failure domain.

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MS108

A Unified Approach on Active Learning Methods for Reliability Analysis

Due to their efficiency in identifying complex failure domains, meta-model-based active learning techniques have been increasingly adopted in the rare events estimation literature. A large number of publications has been devoted in the last decade to capitalizing on the properties of specific surrogate model techniques (*e.g.* Kriging, support vector regression and polynomial chaos expansions) to create adaptive-design strategies that efficiently explore the design space so as to provide stable and accurate estimates of small probability of failure of complex systems. In this contribution, instead of focusing on a specific class of surrogates and rare event estimation techniques (e.g. Monte Carlo simulation or subset sampling), we provide a unified framework to perform adaptive sampling for rare event estimation that does not depend on the specific techniques chosen. This approach can therefore be included in pre-existing workflows with the techniques of choice,

which can be beneficial to increase the appeal of active-learning-based reliability analysis to a wider audience. The performance of the proposed framework is then tested on several benchmark problems by mixing different surrogate-modelling and rare-event-estimation techniques.

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MS108

Rare Event Simulation Through Metamodel-driven Sequential Stochastic Sampling

Rare-event simulation is frequently performed in a sequential setting, introducing a series of intermediate densities that gradually converge to the target one (the rare-event conditional failure density). Subset simulation facilitates, for example, such an approach. For applications with complex numerical models, the associated computational burden for this task is high and the adaptive Kriging stochastic sampling and density approximation algorithm (AK-SSD) is discussed here to alleviate this burden. AKSSD replaces the exact system model with a fast-to-evaluate metamodel, while it also reduces the required number of experiments to construct this metamodel by adaptively adjusting its accuracy through an iterative approach. The metamodel is refined by sample-based design of experiments during this iterative process, such that its prediction ability is improved both globally and locally. Local improvement is sought after in the regions of importance for both the target and the intermediate conditional failure densities. The refinement stops when target densities approximated in consecutive iterations become indifferent, with the Hellinger distance employed as a comparison metric. Once approximated (first stage), the conditional failure density is used (second stage) as importance sampling density for estimating the rare-event likelihood. Use of either the metamodel or the exact numerical model is examined for the second stage.

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MS109

Bayesian Inverse Problems and Low-rank Approximations

We look at Bayesian updating in the framework of updating a random variable (RV) whose distribution is the prior distribution. It is assumed that this RV is a function of many more elementary random variables. Furthermore, it is assumed that computationally the RV is represented in either a sampling format or in a functional or spectral representation like the the polynomila chaos expansion. The samples resp. the coefficients may be viewed as a high degree tensor, and hence it is natural to assume a low-rank approximation for this. Conditioning, the central element of Bayesian updating, is theoretically based on the notion of conditional expectation. Here we use this construct also as the computational basis, namely the ability to compute conditional expectations. With this in hand, we formulate an updating process, which produces a new RV through successively finer approximations, whose law resp. distribution is the sought posterior distribution. This is in effect a kind of filter. It will be shown that it the filter can be computed using low-rank tensor approximations and that it directly operates on the low-rank representation of the RV representing the prior, to produce a low-rank represenatation of the posterior RV.

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MS109

Principal Component Analysis and Active Learning in Tree Tensor Networks

We present an active learning algorithm for the approximation of high-dimensional functions of random variables using tree-based tensor formats (tree tensor networks). The algorithm is based on an extension of principal component analysis to multivariate functions, identified as elements of Hilbert tensor spaces. It constructs a hierarchy of subspaces associated with the different nodes of a dimension partition tree and a corresponding hierarchy of sample-based projection operators. Optimal subspaces are estimated using empirical principal component analysis of partial random evaluations of the function. The algorithm is able to provide an approximation of a function in any tree-based tensor format, with either a prescribed rank or a prescribed relative error, with a number of evaluations of the order of the storage complexity of the resulting tensor network.

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MS109

Multilevel Monte Carlo Computation of Seismic Wave Propagation with Random Lamé Parameters

Abstract not available at time of publication.

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MS109

Sparse Multifidelity Approximations for Forward UQ with Application to Scramjet Combustor Computations

Engineering models of practical interest frequently depend on high-dimensional parameter spaces and the corresponding numerical models are usually computationally expensive. This often limits the number of simulations one can perform and direct explorations of the parameter space are prohibitive. In this talk we discuss progress on constructing lower dimensional surrogate models in a multifidelity setting via sparse regression and adaptive quadrature. We illustrate the algorithms for the analysis of Large Eddy Simulation of a SCRAMJET combustor.

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MS110
Optimization with Fractional PDEs

Fractional differential operators provide an attractive mathematical tool to model effects with limited regularity properties. Particular examples are image processing and phase field models in which jumps across lower dimensional subsets and sharp transitions across interfaces are of interest. In this talk we discuss these applications in addition to optimization problems with PDE constraints. The main emphasis will be on how to account for uncertainty in these models.

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MS110
A Data-oriented Approach to Statistical Inverse Problems

We study a data-oriented (aka consistent) Bayesian approach for inverse problem. Our focus is to investigate the relationship between the data-oriented Bayesian formulation and the standard one for linear inverse problems. We show that 1) from a deterministic point of view, the MAP of the data-oriented Bayesian method is similar to the truncated SVD approach (regularization by truncation), and 2) from the statistical point of view, no matter what prior is used, the method only allows the prior to act on the data uninformed parameter subspace, while leaving the data-informed untouched. Both theoretical and numerical results will be presented to support our approach.

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MS110
Safe Designs via Robust Geometric Programming

Geometric programming is a powerful optimization strategy for an increasingly large class of problems across engineering applications. This work extends geometric programming to the case of optimization under uncertainty. Robust geometric programming helps model and process geometric programs with uncertain data that is known to belong to some uncertainty set. The work presents a methodology to approximate the robust counterparts of an uncertain geometric program as a tractable optimization problem (convex or log-convex) using robust linear programming techniques. This methodology, as well as other existing methodologies, will be used to robustify a complex aircraft design problem, and the results of the different methodologies will be compared and discussed.

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MS110
An Uncertainty-weighted ADMM Method for Multiphysics Parameter Estimation

In this work, we accelerate the convergence of the global variable consensus ADMM algorithm for solving large-scale parameter estimation problems coupling different physics. The idea of global variable consensus is to partition the joint estimation problem into subproblems associated with each PDE, which can be solved individually and in parallel. This allows one to use tailored parameter estimation methods for each problem and is thus attractive for large-scale problems involving complex interactions of multiple physics. A well-known drawback of global variable consensus ADMM is its slow convergence, particularly when the number of workers grows (i.e., a large number of subproblems). To overcome this problem, we propose a new weighting scheme in the algorithm that accounts for the uncertainty associated with the solutions of each subproblem. The uncertainty information can be obtained efficiently using iterative methods, and we demonstrate that the weighting scheme improves convergence for a large-scale multi-physics inverse problem involving a travel time tomography and DC-resistivity survey.

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MS111
Inadequacy Representation of Flamelet-based RANS Model with a Physics-based Stochastic PDE

Stochastic representations of model inadequacy of flamelet-based RANS models for turbulent non-premixed flames are studied. While high fidelity models based on the reacting Navier-Stokes equations are available, turbulent flame simulations based on such models require substantial computational resources and are not practical for use in engineering decision-making. Alternatively, flamelet-based

RANS models introduce a number of simplifying assumptions that lead to dramatically reduced computational cost, but also introduce non-negligible errors. Here, we develop a stochastic modeling approach for representing errors introduced by using assumed PDF for the mixture fraction. Typical deterministic models are based on the mixture fraction mean and variance. We enrich the model by posing a stochastic PDE for the mixture fraction triple correlation. This new state variable is then used to generate perturbations to the assumed PDF, resulting in a stochastic model for all flow variables. A non-premixed hydrogen-air jet flame is used to demonstrate the approach.

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MS111

Bayesian Calibration of Rheological Closure Relations for Computational Models of Turbidity Currents

Numerical models can help to push forward the knowledge about complex dynamic physical systems. The modern approach to doing that involves detailed mathematical models. Turbidity currents are a kind of particle-laden flows that represent a very complex natural phenomenon. In a simple way, they are turbulent driven flows generated between fluids with small density differences carrying particles. They also are one mechanism responsible for the deposition of sediments on the seabed. A detailed understanding of this phenomenon, including uncertainties, may offer new insight to help geologists to understand reservoir formation, a strategic knowledge in oil exploration. We present a finite element formulation applied to the numerical simulation of particle-laden flows in a Eulerian-Eulerian framework. When sediment concentrations are high enough, rheological empirical laws close the model, describing how sediment concentrations influence the mixture viscosity. The aim of this work is to investigate the effects on the flow dynamics of some these empirical laws. We use two configurations for numerical experiments. Both numerical experiments are inspired in laboratory tests. We show how turbulent structures and quantities of interest, such as sediment deposition, are affected by the different empirical rheological laws. Moreover, we employ a Bayesian framework to validate the employed hypothesis and introduce a stochastic error term for taking into account the modeling error.

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MS111

Embedded Model Error Quantification and Propagation

Conventional applications of Bayesian calibration typically assume the model replicates the true mechanism behind data generation. However, this idealization is often not achieved in practice, and computational models frequently carry different physical parameterizations and assumptions than the underlying 'truth'. Ignoring model errors can then lead to overconfident calibrations and predictions around values that are, in fact, biased. Most statistical methods for bias correction are specific to observable quantities, do not retain physical constraints in subsequent predictions, and experience identifiability challenges in distinguishing between data noise and model error. We develop a general Bayesian framework for non-intrusive *embedded* model correction that addresses some of these difficulties, by inserting a stochastic correction to the model input parameters. The physical inputs and correction parameters are then simultaneously inferred. With a polynomial chaos characterization of the correction term, the approach allows efficient quantification, propagation, and decomposition of uncertainty that includes contributions from data noise, parameter posterior uncertainty, and model error. We demonstrate the key strengths of this method on both synthetic examples and realistic engineering applications.

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MS111

Stochastic Inadequacy Models for Chemical Kinetics

Two of the most prominent modeling assumptions used in simulations of turbulent combustion are the introduction of turbulence models and reduced chemistry models. In the present work, we develop a stochastic model inadequacy representation to quantify uncertainties due to reduced models in chemical kinetics. The inadequacy formulation is a generalization of previous work in which a stochastic operator is appended to a reduced chemical kinetics model and calibrated with data from a detailed model using a heirarchical Bayesian approach. The inadequacy formulation accounts for situations in which both reactions and species are neglected from the detailed model. The new inadequacy model was developed to be adaptive such that it is only active when chemical reactions are taking place; otherwise the inadequacy model does not participate. We present results from a perfectly stirred reactor of H_2/O_2 combustion. The detailed model consists of 21 reactions and eight species whereas the reduced model uses five reactions and seven species. We then apply the inadequacy formulation to a one-dimensional counterflow diffusion flame with H_2/O_2 combustion. Finally, we present preliminary results on using the counterflow diffusion flame and its associated uncertainties from the inadequacy formulation to

build an uncertain flamelet library for non-premixed combustion.

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MS112

Emulation of Computer Models with Multivariate Output

Computer models often produce multivariate output. A Gaussian process emulator of a model is typically constructed for each output individually; however, approaches for dependent multivariate emulation of the output have been proposed. We will demonstrate the irrelevance of multivariate modeling of the output of a computer model for the purpose of emulation of the model theoretically and with simulation studies. We will discuss the application of the result to volcano eruption computer models.

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MS112

Sequential Surrogate-based Optimization: Application to Storm Surge Modelling

To mitigate geophysical hazards, it is important to understand the different sources of uncertainty. The computational burden of running a complex computer model, such as a storm surge model, can make optimization and uncertainty quantification tasks impractical. Gaussian Process (GP) regressions are often used as statistical surrogate models to alleviate this issue. They have been shown to be good approximations of the computer model. This study is focused on maximizing an unknown function with the least number of evaluations using the exploration vs. exploitation trade-off strategy: a GP surrogate model is built and employed to achieve this. We explore the uncertain regions and find the input values that maximize the information gain about the function using MICE, a sequential design algorithm which maximizes the mutual information over the input space. The computational efficiency of interweaving MICE and the optimization scheme is examined, and demonstrated on test functions. The benefit of the newly developed sequential surrogate-based optimization scheme is also examined on a storm surge simulator where the aim is to identify conditions that will create possibly large storm surge run-ups at the local level and at the minimum computational cost.

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MS112

Modeling of Geophysical Flows - Analysis of Models and Modeling Assumptions using UQ

Dense large scale granular avalanches are a complex class of flows with physics that has often been poorly captured by models. Sparsity of actual flow data (usually only deposit information is available) and large uncertainty in the mechanisms of initiation and flow propagation make the modeling task challenging and a subject of much continuing interest. Models that appear to represent the physics well in certain flows turn out to be poorly behaved in others due to intrinsic mathematical or numerical issues. While, inverse problems can shed some light on parameter choices it is difficult to make firm judgements on the validity or appropriateness of any single or set of modeling assumptions for a particular target flow or potential flows that needs to be modeled for predictive use in hazard analysis. We will present here an uncertainty quantification based approach to carefully, analyze the effect of modeling assumptions on quantities of interest in simulations based on three established models (Mohr-Coulomb, Pouliqen-Fortere and Voellmy-Salm) and thereby derive a model (from a set of modeling assumptions) suitable for use in a particular context. We also illustrate that a simpler though more restrictive approach is to use a Bayesian modeling average approach based on the limited data to combine the outcomes of different models.

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MS112

Multi-fidelity Sparse-grid-based Uncertainty Quantification Applied to Tsunami Runup

Given a numerical simulation, the objective of parameter estimation is to provide a joint posterior probability distribution for an uncertain input parameter vector, conditional on available experimental data. However, exploring the posterior requires a high number of numerical simulations, which can make the problem impracticable within a given computational budget. A well-known approach to reduce the number of required simulations is to construct a surrogate, which — based on a set of training simulations — can provide an inexpensive approximation of the simu-

lation output for any parameter configuration. To further reduce the total cost of the simulations, we can introduce low-fidelity as well as high-fidelity training simulations. In this case, a small number of expensive high-fidelity simulations is augmented with a larger number of inexpensive low-fidelity simulations. In this talk I will present a multi-fidelity surrogate-based estimator based on sparse grid interpolation. The method will be applied to the quantification of uncertainty for the inundation due to a tsunami runup. We can demonstrate a speedup of 20 for a four dimensional parameter estimation problem.

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MS113

Prediction of Permeability from Digital Images of Reservoir Rocks

Permeability is one of the key petrophysical properties that impact recovery performance of hydrocarbon reservoirs. We introduce a novel Deep Learning system that estimates permeability directly from, SEM, micro-CT, and other Digital Rock images. The core of the system is a convolutional neural network that learns a mapping from the image space to the property space. The trained model predicts properties in seconds, therefore speeding up workflows and complementing/validating laboratory measurements and simulation results, and can also be used as a novel tool for uncertainty quantification. Preliminary results will be presented and discussed.

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MS113

Parametrization and Generation of Geological Models with Generative Adversarial Networks

One of the main challenges in the parametrization of geological models is the ability to capture complex geological structures often observed in subsurface fields. In recent years, Generative Adversarial Networks (GAN) were proposed as an efficient method for the generation and parametrization of complex data, showing state-of-the-art performances in challenging computer vision tasks such as reproducing natural images (handwritten digits, human faces, pets, cars, etc.). In this work, we study the application of Wasserstein GAN for the parametrization of geological models. The effectiveness of the method is assessed for uncertainty propagation tasks using several test cases involving different permeability patterns and subsurface flow problems. Results show that GANs are able to generate samples that preserve the multipoint statistical features of the geological models both visually and quantitatively. The generated samples reproduce both the geological structures and the flow properties of the reference data.

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MS113

Novel Robust Machine Learning Methods for Identification and Extraction of Unknown Features in Complex Real-world Data Sets

Abstract not available at time of publication.

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MS114

Numerical Methods for Hyperbolic Systems of PDEs with Uncertainties

Abstract not available at time of publication.

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MS114

Analysis of UQ in Computational Method for some Kinetic and Hyperbolic Equations

In this talk, I will present some mathematical analysis of UQ in computational method for some kinetic and hyperbolic equations. For neutron transport and radiative transfer equations with small mean free path and random cross-section, we show regularity uniform in random variable and spectral accuracy for gPC Galerkin method. For Burgers equation with shock solution and random initial data, we show that method of polynomial interpolation with proper shifting can capture the physical quantities such as shock emergence time and shock location. This is a joint work with Shi Jin, Qin Li, Zheng Ma, and Ruiwen Shu.

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MS114

Discovering Variable Fractional Orders of Advection-dispersion Equations from Field Data using Multi-fidelity Bayesian Optimization

The fractional advection-dispersion equation (FADE) can describe accurately the solute transport in groundwater but its fractional order has to be determined a priori. Here, we employ multi-fidelity Bayesian optimization to obtain the fractional order under various conditions, and we obtain more accurate results compared to previously published data. Moreover, the present method is very efficient as we use different levels of resolution to construct a stochastic surrogate model and quantify its uncertainty. We consider two different problem set ups. In the first set up, we obtain variable fractional orders of one-dimensional FADE, considering both synthetic and field data. In the second set up, we identify constant fractional orders of two-dimensional FADE using synthetic data. We employ multi-resolution simulations using two-level and three-level Gaussian process regression models to construct the surrogates.

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MS114

Asymptotically Efficient Simulations of Elliptic Problems with Small Random Forcing

Recent rare-event simulations show that the large deviation principle (LDP) for stochastic problems plays an important role in both theory and simulation, for studying rare events induced by small noise. Practical challenges of applying this useful technique include minimizing the rate function numerically and incorporating the minimizer into the importance sampling scheme for the construction of efficient probability estimators. For a spatially extended system where the noise is modeled as a random field, even for simple steady state problems, many new issues are encounteredin comparison to the finite dimensional models. We consider the Poisson'sequation subject to a Gaussian random forcing with vanishing amplitude. In contrast to the simplified rate functional given by space white noise, we consider the covariance operator of trace class such that the effects of small noise of moderate or large correlation length on rare events can be studied. We have constructed an LDP-based importance sampling estimator with a sufficient and necessary condition to guarantee the weak efficiency, where numerical approximation of the large deviation principle is also addressed. Numerical studies have been presented.

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MS115

UQLaB: What's Next?

With the public release of version 1.0, the UQLab project reached a critical maturity stage. This important milestone included the open source release of its scientific modules, in addition to a number of new features, thus marking the beginning of a new development phase in the project. In this contribution we give an overview of the newly introduced scientific modules, which include:

- UQ-Link: a toolbox to easily connect external solvers to the UQLab framework.
- support vector machines (regression + classification) surrogate modelling facilities;
- reliability-based design optimization;
- random fields discretization and sampling.

An outlook to current and upcoming collaborative development efforts will also be presented.

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MS115

QUESO: A Parallel C++ Library for Quantifying Uncertainty in Estimation, Simulation, and Optimisation

QUESO is a tool for quantifying uncertainty for a specific forward problem. QUESO solves Bayesian statistical inverse problems, which pose a posterior distribution in terms of prior and likelihood distributions. QUESO executes MCMC, an algorithm well suited to evaluating moments of high-dimensional distributions. While many libraries exist that solve Bayesian inference problems, QUESO is specialized software designed to solve such problems by utilizing parallel environments demanded by large-scale forward problems. QUESO is written in C++.

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MS115

Integrating SNOWPAC in Dakota with Application to a Scramjet

We present recent developments regarding the integration of SNOWPAC (Stochastic Nonlinear Optimization With Path-Augmented Constraints) in Dakota. SNOWPAC is a method for stochastic nonlinear constrained derivative-free optimization using a trust region approach and Gaussian processes. It solves optimization problems where sampling is used to estimate robustness or risk measures comprising the objective function and/or constraints. We assume that the sample estimates involve expensive black box model evaluations, and thus we focus on a small sample size regime. This introduces significant noise, which slows the optimization process. To mitigate the impact of noise, SNOWPAC employs Gaussian process regression to smooth models of the objective and constraint in the trust region. Additionally, we propose approximate Gaussian process methods in SNOWPAC to handle large numbers of optimization iterations. SNOWPAC is now available in the Dakota framework, which offers a highly flexible interface to couple the optimizer with different sampling strategies or surrogate models. In this presentation we give details about SNOWPAC and show the coupling of the libraries. Finally, we showcase the approach by presenting design optimization results on a challenging scramjet application. Here, Dakota serves as the driver of the optimization process, employing SNOWPAC as optimization method and

multilevel Monte Carlo sampling to evaluate the robustness measures.

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MS115

Markov Chain Monte Carlo Sampling using GPU Accelerated Sparse Grids Surrogate Models

We combine the DiffeRential Evolution Adaptive Metropolis (DREAM) algorithm to surrogate models constructed using sparse grids (SG) approximation. DREAM allows us to collect random samples form a general probability distribution, the algorithm can be used to solver problems of Bayesian inference and multidimensional optimization. The challenge of the approach comes form the very large number of DREAM samples needed to compute reliable statistics, which in turn requires a very large number of SG evaluations. The DREAM algorithm processes samples in batches, and the corresponding SG evaluation consists of two stages: first, construct a matrix of function values that is either sparse or dense (depending on the type of SG used); second, multiply the matrix by a precomputed data matrix. We present a comparison of different ways to accelerate both stages of the computation using Nvidia GPUs and leveraging the accelerated libraries cuBLAS and cuSparse, the newly developed capabilities in in Matrix Algebra on GPU and Multicore Architectures, as well as custom CUDA kernels. We show benchmark results from several hardware architectures and GPU generations.

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MS116

Numerical Methods for Stochastic Delay Differential Equations under Non-global Lipschitz Condition

A class of explicit balanced schemes is presented for stochastic delay differential equations under some non-global Lipschitz conditions. One scheme is a balanced Euler scheme, which is proved to be of order half in mean-square sense, another one is a balanced Milstein scheme with first-order convergence. Numerical stability of the two presented schemes is further considered. Some numerical examples are given to verify our theoretical predictions.

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MS116

Stochastic Computational Singular Perturbation for Complex Chemical Reaction Systems

The research on reduction methods for chemical reaction systems is driven by their complexity, to seek simplified systems involving a smaller set of species and reactions that can approximate the original detailed systems in the prediction of specific quantities of interest. The existence of such reduced systems frequently hinges on the existence of a lower-dimensional, attracting, and invariant manifold characterizing long-term dynamics. The Computational Singular Perturbation (CSP) method provides a general framework for analysis and reduction of chemical reaction systems, but is not directly applicable to chemical reaction systems at micro or mesoscale, where stochasticity plays a non-negligible role and thus has to be taken into account. In this presentation a stochastic computational singular perturbation method and associated algorithm will be presented. They can be used to not only construct accurately and efficiently the numerical solutions to stiff stochastic chemical reaction systems, but also analyze the dynamics of the reduced stochastic reaction systems.

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MS116

Chemical Reaction Noise Induced Phenomena: Change in Dynamics and Pattern Formation

It has been realized that noise can have an effect on reaction diffusion systems. In particular, including noise in reaction diffusion models can induce pattern formation or change the patterns in the deterministic models. In this talk, I will provide a method for analyzing such effects from intrinsic chemical reaction noise. I will first provide a framework for understanding how chemical reaction noise can change the systems' effective dynamics. Then the approach will be applied to the classical Gray-Scott model and a quantitative analysis of noise induced phenomena will be elaborated and compared to the numerical simulations.

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MS116

Efficient Integration of Fractional Beam Equation with Space-time Noise

We consider numerical solutions of a nonlinear Beam equation driven by space-time white noise with time-fractional derivative. The solution of the considered equations require large storage and prohibitively computational cost. To al-

leviate heavy computational cost and storage requirement, we employ low-cost and low-storage fast algorithms to solve the problem. We apply an implicit-explicit scheme and reduce the problem to a system of linear time-fractional differential equation which can be solved efficiently. The proposed method significantly improve a method developed in literature.

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MS117

Importance Sampling the Union of Rare Events with Bounded Relative Error and an Application to Power Systems Analysis

This work presents a method for estimating the probability μ of a union of J rare events. The method uses n samples, each of which picks one of the rare events at random, samples conditionally on that rare event happening and counts the total number of rare events that happen. We call it ALORE, for 'at least one rare event'. The ALORE estimate is unbiased and has a coefficient of variation no larger than $\sqrt{(J + J^{-1} - 2)/(4n)}$. The coefficient of variation is also no larger than $\sqrt{(\bar{\mu}/\mu - 1)/n}$ where $\bar{\mu}$ is the union bound. Our motivating problem comes from power system reliability, where the phase differences between connected nodes have a joint Gaussian distribution and the J rare events arise from unacceptably large phase differences. In the grid reliability problems even some events defined by 5772 constraints in 326 dimensions, with probability below 10^{-22}, are estimated with a coefficient of variation of about 0.0024 with only $n = 10{,}000$ sample values.

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MS117

Input-output Uncertainty Comparisons for Optimization via Simulation

When input distributions to a simulation model are estimated from real-world data, they have estimation error causing input uncertainty in the simulation output. If an optimization via simulation (OvS) method that treats such input distributions as 'correct' is applied, then there is a risk of making a suboptimal decision for the real world, which we call input model risk. This talk addresses the discrete OvS (DOvS) problem of selecting the real-world optimal from among a finite number of systems when all of them share the same input distributions estimated from common input data. A DOvS procedure should reflect the limited resolution provided by the simulation model in distinguishing the real-world optimal solution from the others when the input data are finite. Our input-output uncertainty comparisons (IOU-C) procedure focuses on comparisons rather than selection: it provides simultaneous confidence intervals for each systems real-world mean and the best mean of the rest with any desired probability, while accounting for both stochastic and input uncertainty. To make the resolution as high as possible (intervals as short as possible) we exploit the common input data effect to reduce uncertainty in the estimated differences. Under mild conditions we prove that the IOU-C procedure provides the desired statistical guarantee asymptotically as the real-world sample size and simulation effort increase, but it is designed to be effective in finite samples.

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MS117

Universal Convergence of Kriging

Kriging based on Gaussian random fields is widely used in reconstructing unknown functions. The kriging method has pointwise predictive distributions which are computationally simple. However, in many applications one would like to predict for a range of untried points simultaneously. In this work we obtain some error bounds for the (simple) kriging predictor under the uniform metric. It works for a scattered set of input points in an arbitrary dimension, and also covers cases where the covariance function of the Gaussian process is misspecified. These results lead to a better understanding of the rate of convergence of kriging under the Gaussian or the Matérn correlation functions, the relationship between space-filling designs and kriging models, and the robustness of the Matérn correlation functions.

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MS117

Experimental Designs for Uncertainty Propagation and Robustness Analysis

For an input-output system, uncertainty propagation studies how variability in input variables (e.g., resulting from manufacturing tolerances) affect the variability in output variables. For real-world engineering problems, this input-output system is typically black-box and requires simulations to evaluate; in such situations, uncertainty propagation is performed by pushing-forward a set of input settings through a simulator. Since each simulation run can be computationally or monetarily expensive, the goal is to reduce the number of runs needed to conduct this propagation. In this talk, we present a novel experimental design approach, which makes use of a designed set of inputs to perform this propagation using a limited number of samples. The proposed design is shown to perform better than Monte Carlo and Quasi-Monte Carlo samples. We illustrate the effectiveness of the proposed designs in numerical simulations, and demonstrate its usefulness in several real-world applications such as robust parameter design of a product or

process.

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MS118

Uncertainty Quantification of Transport in Heterogeneous Porous Media with the Iruq-Cv Method

We present an inverse regression-based approach for uncertainty quantification with application to solute transport in heterogeneous porous media. In the proposed approach we used sliced inverse regression (SIR) to identify a dimension reduction subspace of random space that sufficiently captures the variability of the quantities of interest (QoIs) under consideration. This dimension reduction subspace is then employed to construct a surrogate model for the QoI by means of Hermite polynomial expansions. Estimates of statistics of QoIs are computed by using the surrogate model as a control variate, reducing the error of the estimates. We consider solute transport problems in saturated media, where the hydraulic conductivity field is modeled as a second-order random field. We apply the proposed approach to the estimation of statistics of the maximum concentration and mean arrival time at various observation locations throughout the simulation domain.

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MS118

Efficient Stochastic Inversion Using Adjoint Models and Machine Learning

Performing stochastic inversion on a computationally expensive forward simulation model with a high-dimensional uncertain parameter space (e.g. a spatial random field) is computationally prohibitive even when gradient information can be computed efficiently. Moreover, the 'nonlinear' mapping from parameters to observables generally gives rise to non-Gaussian posteriors even with Gaussian priors, thus hampering the use of efficient inversion algorithms designed for models with Gaussian assumptions. In this paper, we propose a novel Bayesian stochastic inversion methodology, which is characterized by a tight coupling between the gradient-based Langevin Markov Chain Monte Carlo (LMCMC) method and a kernel principal component analysis (KPCA). This approach addresses the 'curse-of-dimensionality' via KPCA to identify a low-dimensional feature space within the high-dimensional and nonlinearly correlated parameter space. In addition, non-Gaussian posterior distributions are estimated via an efficient LMCMC method on the projected low-dimensional feature space. We will demonstrate this computational framework by integrating and adapting our recent data-driven statistics-on-manifolds constructions and reduction-through-projection techniques to a linear elasticity model. 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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MS118

Compressive Sensing with Built-in Basis Adaptation for Reduced Homogeneous Chaos Expansions

Compressive sensing methods have recently gained increasing momentum in the context of polynomial chaos expansions with an emphasis on its applicability in computationally expensive or high dimensional models. We present a novel heuristic algorithm that utilizes such methods in order to compute optimal adapted bases in Homogeneous Chaos spaces. This consists of a two-step optimization procedure that computes the coefficients and the input projection matrix of a low dimensional chaos expansion with respect to a rotated basis. We demonstrate the attractive features of our algorithm through several numerical examples including the application on Large-Eddy simulations of turbulent combustion in a HiFiRE scramjet engine.

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MS119

Random Sketching for Model Order Reduction of High Dimensional Systems

We propose a methodology for reducing the cost of the classical projection based Model Order Reduction algorithms while preserving the quality of the output. We show that to build the surrogate model it is enough to consider a sketch of the full problem, i.e. a set of low-dimensional projections, instead of operating on large matrices and vectors. A sketch is computed randomly and guaranteed to contain the key information with high probability. Our approach can be used for reducing both complexity and memory. The algorithms provided here are well suited for any modern computational environment. All the operations, except solving linear systems of equations, are embarrassingly parallel. Our version of Proper Orthogonal Decomposition can be computed on separate machines with a communication cost independent of the dimension of the full problem. The surrogate model can even be constructed in the so-called streaming environment, i.e., under extreme memory constraints. In addition, we provide an efficient way for estimating the residual norm. This approach is not only more efficient than the classical one but is also less sensitive to round-off errors. Finally, we validate the methodology nu-

merically on a benchmark problem.

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MS119

Gradient-free Active Subspace Techniques to Construct Surrogate Models Employed for Bayesian Inference

Physical models employed in neutronics, thermal hydraulics, fuels and chemistry codes typically have a moderate (10-100) or high (> 100) number of inputs – comprised of parameters, initial or boundary conditions, or exogenous forces – many of which are nonidentifiable or noninfluential in the sense that they are not uniquely determined by the data. We demonstrate the use of a novel initialization algorithm to approximate the gradients used to construct active subspaces for neutronics, thermal hydraulics, fuels and chemistry models with moderate input dimensions. We subsequently construct surrogate models on these active subspaces, which can be used for subsequent analysis, model calibration via Bayesian inference, or uncertainty quantification.

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MS119

Certified Reduced Basis Methods for Variational Data Assimilation

The reduced basis (RB) method is a certified MOR technique for the rapid and reliable solution of parametrised PDEs. Here, we focus on problems in optimal control and data assimilation. In particular, we present a certified RB approach to four dimensional variational data assimilation (4D-Var). Several works have explored the use of reduced order models as surrogates in a 4D-Var setting. We consider the case in which the behavior of the system is modelled by a parametrised parabolic PDE where the initial condition and model parameters (e.g., material or geometric properties) are unknown, and where the model itself may be imperfect. We consider (i) the standard strong-constraint 4D- Var approach, which uses the given observational data to estimate the unknown initial condition of the model, and (ii) the weak-constraint 4D-Var formulation, which additionally provides an estimate for the model error, and thus can deal with imperfect models. Since the model error is a distributed function in both space and time, the 4D-Var formulation generally leads to a large-scale optimization problem that must be solved for every given parameter instance. We introduce RB spaces for the state, adjoint, initial condition, and model error. We then build upon recent results on RB methods for optimal control problems to derive a posteriori error estimates for RB approximations to solutions of the 4D-Var problem. Numerical tests are conducted to verify the validity of the proposed approach.

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MS119

Dictionary Measurement Selection for State Estimation with Reduced Models

Parametric PDEs of the general form

$$\mathcal{P}(u, a) = 0$$

are commonly used to describe many physical processes, where $\mathcal{P}$ is a differential operator, a is a high-dimensional vector of parameters and u is the unknown solution belonging to some Hilbert space V. Typically one observes m linear measurements of $u(a)$ of the form $\ell_i(u) = \langle w_i, u\rangle$, $i = 1, \dots, m$, where $\ell_i \in V'$ and w_i are the Riesz representers, and we write $W_m = \text{span}\{w_1, \dots, w_m\}$. The goal is to recover an approximation u^* of u from the measurements. The solutions $u(a)$ lie in a manifold within V which we can approximate by a linear space V_n, where n is of moderate dimension. The structure of the PDE ensure that for any a the solution is never too far away from V_n, that is, $\text{dist}(u(a), V_n) \leq \varepsilon$. In this setting, the observed measurements and V_n can be combined to produce an approximation u^* of u up to accuracy

$$\|u - u^*\| \leq \beta^{-1}(V_n, W_m)\,\varepsilon$$

where

$$\beta(V_n, W_m) := \inf_{v \in V_n} \frac{\|P_{W_m} v\|}{\|v\|}$$

plays the role of a stability constant. For a given V_n, one relevant objective is to guarantee that $\beta(V_n, W_m) \geq \gamma > 0$ with a number of measurements $m \geq n$ as small as possible. We present results in this direction when the measurement functionals ℓ_i belong to a complete dictionary.

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MS120

Opportunities and Unsolved Problems in Quantifying Seemingly Random Behavior in Images of Shock Waves

Images of shock waves show irreproducible, stochastic and inhomogeneous behavior that is caused by material dynamics that are just beyond what state-of-the-art experiments can resolve. While statistical models describing the variation and uncertainty in these images could inform the underlying physics, much of that analysis is missing. Shock images typically have an assortment of noise, intensity variation, low contrast, blur, and other quality issues from experimental constraints, which cause most conventional analysis methods to fail. These data-rich images usually remain un-analyzed because few experimentalists have the expertise to develop new methods to accommodate these constraints. As an experimentalist, I will present a variety of different types of image data that will show the scope of statistical uncertainty shown in images of shock phenomena. This talk will give an overview of the unsolved problems in UQ that are currently in high-demand for the shock physics community. I will touch on possibilities in digital image correlation, image segmentation, texture analysis, gradient methods, as well as model-based analysis, and other fields beyond.

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MS120

A Locally Adapting Technique for Quantifying Error in Boundary Locations using Image Segmentation

To compute quantities such as pressure and velocity from laser-induced shock waves propagating through materials, high-speed images are captured and analyzed. Shock images typically display high noise and spatially-varying intensities, causing conventional analysis techniques to have difficulty identi- fying boundaries in the images without making significant assumptions about the data. We present a novel machine learning algorithm that efficiently segments, or partitions, images with high noise and spatially-varying intensities, and provides error maps that describe a level of uncertainty in the partition- ing. The user trains the algorithm by providing locations of known materials within the image but no assumptions are made on the geometries in the image. The error maps are used to provide lower and upper bounds on quan- tities of interest, such as velocity and pressure, once boundaries have been identified and propagated through equations of state. This algorithm will be demonstrated on images of shock waves with noise and aberrations to quantify properties of the wave as it progresses. This work was done by National Security Technologies, LLC, under Contract No. DE- AC52-06NA25946 with the U.S. Department of Energy and supported by the Site-Directed Research and Development Program.

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MS120

Radially Symmetric Modeling for Large Scale Linear Inverse Problems in X-ray Imaging

In several applications of X-ray imaging, quantitative estimation incorporates an assumption of radial symmetry. The dimensionality of the quantity of interest is often reduced, e.g. a two-dimensional image of a radially symmetric object can be represented with its radial profile, but assumptions about the object must now be translated appropriately to reflect the geometry of the *radial profile*. With the Bayesian viewpoint, this can be implemented by modeling the prior with radial symmetry. In particular, this work shows how radial symmetry can be incorporated into Markov field prior distributions whose precision is a high dimensional approximation to a differential operator. We show how these types of priors can be used for estimation problems on actual X-ray radiographic data, such as estimating the point spread function of the system or recovering areal density through Abel inversion.

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MS120

Fast Experimental Designs for LARGE Linear Processes

Microbial biofilms are virtually everywhere, exploiting sources of chemical and photo energy wherever they can be found. A deeper understanding of their function can profoundly transform the way we understand and interact with our world. Microbiologists have unprecedented access to inexpensive molecular metagenomic, metatranscriptomic and imaging technologies that has revolutionized the potential to identify and characterize microbial community capability and activity. At the same time increasingly sophisticated microprobe and imaging technology has enabled resolution, down to the microscale, of the environment in which microbial communities function. Community scale mathematical models of microbial communities are also available and capable of describing the interaction between these disparate biological and chemical and physical data. Our goal is to understand both the forward (omics to environmental) and backward (environment to omics) processes through efficient experimental designs that generate laboratory data that optimally inform the underlying mathematical model.

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MS121

Continuous Level Monte Carlo and Sample-adaptive Model Hierarchies

In this talk, we present Continuous Level Monte Carlo (CLMC), a generalisation of Multilevel Monte Carlo (MLMC) to a continuous framework where the level parameter is a continuous variable. This provides a natural framework to use sample-wise adaptive refinement strategies, with a goal-oriented error estimator as our new level

parameter. We introduce a practical CLMC estimator (and algorithm) and prove a complexity theorem showing the same rate of complexity as MLMC. Also, we show that it is possible to make the CLMC estimator unbiased with respect to the true quantity of interest. Finally, we provide two numerical experiments which test the CLMC framework alongside a sample-wise adaptive refinement strategy, showing clear gains over a standard MLMC approach.

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MS121

An Efficient Algorithm for a Class of Stochastic Wave Propagation Models

We consider a class of frequency domain stochastic wave propagation models in heterogeneous media, with uncertainty in the output propagation quantities of interest (QoI) induced by random parameters describing the heterogeneity. We compute high-order approximations to stochastic moments of the QoI using an efficient high-dimensional parameter sampling technique.

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MS121

Efficient Sampling from High-dimensional Distributions using Low-rank Tensor Surrogates

High-dimensional distributions are notoriously difficult to sample from, particularly in the context of PDE-constrained Bayesian inverse problems. In this talk, we will present general purpose samplers based on low-rank tensor surrogates in the tensor-train (TT) format, a methodology that has been exploited already for many years for scalable, high-dimensional function approximations in quantum chemistry. In the Bayesian context, the TT surrogate is built in a two stage process. First we build a surrogate of the entire PDE solution in the TT format, using a novel combination of alternating least squares and the TT cross algorithm. It exploits and preserves the block diagonal structure of the discretised operator in stochastic collocation schemes, requiring only independent PDE solutions at a few parameter values, thus allowing the use of existing high performance PDE solvers. In a second stage, we approximate the high-dimensional likelihood function also in TT format. Due to the particular structure of the TT surrogate, we can build an efficient inverse Rosenblatt (or cumulative) transform that only requires a sampling algorithm for one-dimensional conditionals. The overall computational cost of the sampler grows only linearly with the dimension. For sufficiently smooth prior distributions of the input random fields, the ranks required for accurate TT approximations are moderate, leading to significant computational gains.

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MS121

A High-performance Software Framework for Multilevel Uncertainty Quantification

A common technique for solving Bayesian inference problems is the Markov Chain Monte Carlo (MCMC) algorithm. However, in engineering applications the inference problem is typically constrained by partial differential equations (PDEs), requiring the costly numerical solution of a PDE in every single step of the chain. Many of the samples are subsequently discarded. Clearly, for large problems this leads to a massive computational effort. In analogy to multilevel PDE solvers, the Multilevel Markov Chain Monte Carlo (MLMCMC) method exploits the structure within the underlying PDE in order to carry out the inference at a fraction of the computational cost of classical methods. It restricts most of the sampling effort to easy-to-compute coarse approximations of the PDE, while requiring only a small number of realisations at full accuracy. In this talk we give an algorithmic view of the MLMCMC approach, as well as describing a new implementation that leverages both the high-performance PDE library DUNE (https://www.dune-project.org/) and a new extension to the MIT Uncertainty Quantification library MUQ (http://muq.mit.edu/). The former is an efficient modular library for solving large-scale PDEs in high performance computing environments, while the latter provides an easy-to-use framework to handle the statistical part of the method, including cutting-edge proposal distributions. We demonstrate the effectiveness of the new implementation on a number of applications.

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MS122

Adaptive Tensor Methods for Forward and Inverse Problems

Abstract not available at time of publication.

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MS122

Low-rank Tensors for Stochastic Forward Problems

Abstract not available at time of publication.

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MS122

Sparse Spectral Bayesian Estimation of Nonlinear Mechanical Models

In this paper we study the uncertainty quantification in a functional approximation form of nonlinear mechanical models parametrised by material uncertainties. Departing from the classical optimisation point of view, we take a slightly different path by solving the problem in a Bayesian manner with the help of new spectral based sparse Kalman filter algorithms. The identification employs the low-rank structure of the solution and provides the confidence intervals on the estimated solution.

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MS122

Bayesian Estimation for a Tomography Problem

We use Bayesian estimation for a tomography problem modeled by a partial differential equation, where randomness is due to the uncertainty in the quantity of interest. The Poisson-Boltzmann equation is the main model equation solved on a bounded and convex domain and applications include electric-impedance tomography as well as nanoscale field-effect sensors. The unknown quantity of interest is the permittivity describing the size, number, and location of target molecules or inclusions; the goal is to identify these parameters. We use the Metropolis-Hastings algorithm in the context of Markov-chain Monte-Carlo (MCMC) methods to estimate the posterior distribution of the size, number, and location of the inclusions as the quantity of interest in our model problem. The MCMC method is computationally expensive and requires the calculation of the model response for a large number of samples (at least tens or hundreds of thousands), for each of which the PDE model must be solved. Thus, an iterative MCMC solver helps to improve efficiency. This means we estimate the posterior distribution for the parameters of interest and then using this distribution as the prior estimation, we estimate another posterior in the next iteration. The trade-off between the number of iterations and the number of samples used in each iteration is discussed and results for a realistic problem are shown.

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MS123

Calibration and Multi-stage Emulation for Disaggregation and Complex Models

Uncertainty quantification methods are often useful for multi-scale problems. This talk will give an overview of some of the broad challenges in uncertainty quantification for multi-scale systems. Some of the broad challenges may include calibration of a large parameter space, development of a multi-stage emulator, handling model discrepancy, experimental design, and computational challenges. These challenges will be discussed using a couple different applications. One is the disaggregation of a complex target, in this example to determine the chemical composition using laser induced breakdown spectrography (LIBS) measurements and output from a complex forward model. The second application is the calibration of a multi-scale solvent-based carbon capture model to obtain accurate predictions of the proportion of carbon captured.

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MS123

Parameter Estimation for System Submodels with Limited or Missing Data using a Data-free Inference Procedure

Predictive simulations of real-world systems often employ physics-based submodels whose parameters are constrained by comparison to experimental data. Since raw experimental data are typically unreported, the form in which summary statistics of the data in the form of parameters and their uncertainties is presented is crucial for enabling statistical analyses, such as uncertainty quantification (UQ) and uncertainty propagation. In order to explore the joint parametric uncertainty structure for submodels in cases where supporting data is limited or missing, we construct a data inference procedure which employs the available information as constraints to explore a space of hypothetical noisy data consistent with these constraints. The algorithm involves nested Bayesian inferences on data and parameters respectively, employing a maximum entropy approach with Approximate Bayesian Computation (ABC) to enforce consistency though a data likelihood function. The algorithm delivers consistent noisy data sets and associated joint parameter densities, which can be pooled to arrive at a consensus density. This approach both facilitates UQ in the absence of data evidence, and also proposes a framework for data assimilation across separate experiments and their potentially varying reporting paradigms using a universal data-centric representation of experimental evidence and uncertainty.

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MS123

Dynamic Discrepancy: Intrusive Methods for Getting More Science into Industrial Models

Complex physical phenomena often require equally complex models to describe them. Incorporating these high-order models into large-scale models of industrial systems is a persistent challenge. This presentation will provide an introduction to dynamic discrepancy reduced modeling, in which relatively simple dynamic models arising from physical systems are outfitted with Gaussian process (GP) stochastic functions of the BSS-ANOVA type. Advantageous properties of the BSS-ANOVA GP render such models particularly suited for Bayesian calibration to data generated by experiment, by high-fidelity models or both. Selected applications will focus on the chemical engineering sector, to include carbon capture and catalytic steam reformation. The potential for machine learning through automated model building will be discussed.

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MS124

Model Error Treatment in Data Assimilation for High-dimensional System - The Environmental Prediction Case

In this talk, I will first briefly describe the general issue of model error treatment in data assimilation (DA) for high-dimensional chaotic dynamics, such as those encountered in environmental prediction. Emphasis will be given to ensemble-based DA methods. A novel approach, in which model error is treated as a deterministic process correlated in time, will be discussed in the second part. This allows for the derivation of the evolution equations for the relevant moments of the model error statistics required in DA, along with an approximation suitable for application to large numerical models. It will be shown how this deterministic description of the model error can be incorporated in sequential and variational DA procedures. A numerical comparison with standard methods is given using low-order dynamical systems, prototypes of atmospheric circulation, and a realistic soil model. In the final part of the talk I will summarize methods for estimating the statistical inputs of the model error, in relation but not limited to the deterministic approach discussed before. A novel procedure based on combining the ensemble Kalman filter with expectation-maximization and Newton-Raphson maximum likelihood methods will be presented.

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MS124

Impact of Model Fidelity on Bayesian Experimental Design

Accurate parameter estimation of a physical system is crucial to many engineering applications; this can be achieved in a stochastic manner through Bayesian inference. However, the available data might not be sufficient to accurately inform all model parameters. It is therefore desirable to design experiments, using a simulation code, that maximize the amount of information that can be extracted from the data. Bayesian Experimental Design is a novel strategy for accomplishing this goal. Reducing the computational cost, especially to evaluate the associated utility functions is of critical importance, and has attracted considerable interest in recent years. One area that has not been explored in depth is the impact of model inadequacy on the results of the experimental design. To this end, we test Bayesian Experimental Design on a hierarchy of nonlinear models for some test problems in fluid dynamics. We investigate the sensitivity of the optimal experimental design points as a function of model choice, and compare the resulting posterior parameter distributions.

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MS124

Scalable Parallel Solution and Uncertainty Quantification Techniques for Variational Inference

Data assimilation (DA) uses physical measurements along with a physical model to estimate the parameters or state of a physical system. Solution to DA problems using the variational approach require multiple evaluations of the associated cost function and gradient. In this work we present a scalable algorithm based on augmented Lagrangian approach to solve the 4D-Var. The augmented Lagrangian framework facilitates parallel evaluation of cost function and gradients. We show that this methodology is scalable with increasing problem size by applying it to the Lorenz-96 model and the Shallow Water model. We also develop a systematic framework to quantify the impact of observation and model errors on the solution to the 4D-Var. We demonstrate this a-posteriori error estimation framework on the weather research and forecast (WRF) model.

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MS124

Reducing Model Discrepancies in Turbulent Flow Simulations with Physics-informed Machine Learning

Turbulence modeling introduces large model-form uncertainties in the predictions. Recently, data-driven methods have been proposed as a promising alternative by using existing database of experiments or high-fidelity simulations. In this talk, we present a physics-informed machine-learning-assisted turbulence modeling framework. This framework consists of three components: (1) reconstructing Reynolds stress modeling discrepancies based on DNS data via machine learning techniques, (2) assessing the prediction confidence a priori based on distance metrics in the mean flow features space, and (3) propagating the predicted Reynolds stress field to mean velocity field by using physics-informed stabilization. Several flows with massive separations are investigated to evaluate the performance of the proposed framework. Significant improvements over the baseline RANS simulation are observed for the Reynolds stress and the mean velocity fields.

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MS125

Bayesian Inversion of Volcano Monitoring Data using Physics-based Eruption Models

Monitoring data such as gas emission rates, ground surface deformation, and rock geochemistry are routinely collected at many volcanoes. Utilizing these evolving observations to characterize volcano source parameters (magma reservoir volume, pressure, composition, etc.) and associated uncertainties is critical for basic science and for hazard monitoring, forecasting, and mitigation, but remains a significant challenge. Here I discuss the use of physics-based eruption models in a Bayesian framework to jointly invert diverse monitoring data in order to resolve probabilistic volcanic source properties and, in limited cases, forecast future behavior. This approach has yielded otherwise difficult-to-obtain insights into volcanic systems, including magmatic volatile content and reservoir volume at Mount St. Helens (Washington), magma supply rate and composition at Kilauea Volcano (Hawaii), and even insight into the mantle regions which feed eruptions. Ongoing challenges include physical processes that are often poorly understood and occur over a wide range of spatial and temporal scales, volcano models that may be computationally expensive and exhibit multiple solutions for a given set of model parameters, and inadequately resolved data uncertainties.

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MS125

Practical Heteroskedastic Gaussian Process Regression

We present a unified view of likelihood based Gaussian progress regression for simulation experiments exhibiting input-dependent noise. Replication plays an important role in that context, however previous methods leveraging replicates have either ignored the computational savings that come from such design, or have short-cut full likelihood-based inference to remain tractable. Starting with homoskedastic processes, we show how multiple applications of a well-known Woodbury identity facilitate inference for all parameters under the likelihood (without approximation), bypassing the typical full-data sized calculations. We then borrow a latent-variable idea from machine learning to address heteroskedasticity, adapting it to work within the same thrifty inferential framework, thereby simultaneously leveraging the computational and statistical efficiency of designs with replication. The result is an inferential scheme that can be characterized as single objective function, complete with closed form derivatives, for rapid library-based optimization. Illustrations are provided, including real-world simulation experiments from manufacturing and the management of epidemics.

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MS125

An Improved Approach to Imperfect Computer Model Calibration and Prediction

We consider the problem of calibrating inexact computer models using experimental data. To compensate for the misspecification of the computer model, a discrepancy function is usually included and modeled via a Gaussian stochastic process (GaSP), leading to better results of prediction. The calibration parameters in the computer model, however, sometimes become unidentifiable in the GaSP model, and the calibrated computer model fits the experimental data poorly as a consequence. In this work, we propose the scaled Gaussian stochastic process (S-GaSP), a novel stochastic process for calibration and prediction. This new approach bridges the gap between two predominant methods, namely the L_2 calibration and GaSP calibration. A computationally feasible approach is introduced for this new model under the Bayesian paradigm. The S-GaSP model not only provides a general framework for calibration, but also enables the computer model to predict well regardless of the discrepancy function. Numerical examples are also provided to illustrate the connections and differences between this new model

and other previous approaches.

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MS125

Multi-objective Sequential Design for Hazard Mapping

Output from computer simulations of geophysical mass flows often has a complicated, topography dependent spatial footprint. If we consider the hazard threat at one map point, emulators can be used to aid in identifying key regions of input space in which to focus sampling for calculating the probability of the hazard threat and to quantify uncertainties of those calculations. You could imagine repeating this process for another map point and identifying a very different important region of input space for that new location. This leads to a challenge if we need to produce maps quickly and/or have a limited compute budget. Effectively, if we seek to add additional design points or batches of design points, there will be multiple objectives to satisfy corresponding to different regions of the map. We will present a multi-objective design strategy and demonstrate it on probabilistic hazard mapping for the Long Valley volcanic region.

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MS126

Fitting Dynamic Models to Epidemic Outbreaks with Quantified Uncertainty: Parameter Uncertainty, Identifiability, and Forecasts

Mathematical models provide a quantitative framework with which scientists can assess hypotheses on the potential underlying mechanisms that explain patterns in observed data at different spatial and temporal scales, generate estimates of key kinetic parameters, assess the impact of interventions, optimize the impact of control strategies, and generate forecasts. We review and illustrate a simple data assimilation framework for calibrating mathematical models based on ordinary differential equation models using time series data describing the temporal progression of case counts relating, for instance, to population growth or infectious disease transmission dynamics. In contrast to Bayesian estimation approaches that always raise the question of how to set priors for the parameters, this frequentist approach relies on modeling the error structure in the data. We discuss issues related to parameter identifiability, uncertainty quantification and propagation as well as model performance and forecasts along examples based on phenomenological and mechanistic models parameterized using simulated and real datasets.

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MS126

Implications of Uncertainty in Parameter Estimation for a Biomthematical Based Response Metric for Glioblastoma

Glioblastomas, a type of lethal primary tumor, are known for their heterogeneity and invasiveness. Over the last decade, a growing literature has been developed demonstrating the clinical relevance of a biomathematical model, the Proliferation-Invasion (PI) model, of glioblastoma growth in giving patient-specific insight into the individual tumor kinetics. Of specific interest to this work, is the development of a treatment response metric, the Days Gained (DG) metric, based on individual tumor kinetics estimated through the PI model using segmented volumes of hyperintense regions on T1-weighted enhanced with gadolinium and T2-weighted magnetic resonance images from two time points. This metric was shown to be more prognostic of outcome than standard imaging response metrics for a cutoff of DG=91. The original papers considered a cohort of 63 patients, but did not account for the various types of uncertainty in the calculation of the DG metric leaving the robustness of this cutoff and metric in question. In this work, we harness the Bayesian framework to consider two sources of uncertainty coming from image acquisition and the interobserver error in image segmentation. Our results show that while the uncertainty can result in relatively large confidence intervals for the DG metric in individual patients, the previously suggested cutoff of 91 days remains robust. This supports the use of the single value of DG as a clinical tool.

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MS126

Data Assimilation and Parameter Identification in a Dynamical Model of Cancer Treatment

This talk provides an overview of some of the issues that arise when trying to validate a biomathematical model from data. I will describe some ordinary differential equation models of prostate cancer growth and its treatment by hormone (androgen deprivation) therapy. Although such therapy usually is quite effective initially, the tumor inevitably evolves resistance. The underlying biological mechanisms of treatment resistance are complex, and researchers have proposed various simplifications in attempts to derive tractable mathematical models of treatment response. One objective of such modeling efforts is to determine, based on time series data of tumor markers such as serum concentrations of prostate-specific antigen, whether the tumor has evolved resistance (or soon will do so). Attempts to answer this question involve matters of model and measurement error and the identifiability of key model parameters.

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MS126

Sub-exponential Growth for Modeling Plague: A Case Study of the 1904 Bombay Plague

Abstract not available at time of publication.

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MS127

Applying Quasi-Monte Carlo to an Elliptic Eigenvalue Problem with Stochastic Coefficients

In this talk we study an elliptic eigenvalue problem, with a random coefficient that can be parametrised by infinitely-many stochastic parameters. The physical motivation is the criticality problem for a nuclear reactor: in steady state the fission reaction can be modelled by an elliptic eigenvalue problem, and the smallest eigenvalue provides a measure of how close the reaction is to equilibrium – in terms of production/absorption of neutrons. The coefficients are allowed to be random to model the uncertainty of the composition of materials inside the reactor, e.g., the control rods, reactor structure, fuel rods etc. The randomness in the coefficient also results in randomness in the eigenvalues and corresponding eigenfunctions. As such, our quantity of interest is the expected value, with respect to the stochastic parameters, of the smallest eigenvalue, which we formulate as an integral over the infinite-dimensional parameter domain. Our approximation involves three steps: truncating the stochastic dimension, discretising the spatial domain using finite elements and approximating the now finite but still high-dimensional integral. To approximate the high-dimensional integral we use quasi-Monte Carlo methods. We show that the minimal eigenvalue belongs to the spaces required for QMC theory, outline the approximation algorithm and provide numerical results.

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MS127

Recursive Numerical Integration for Lattice Systems with Low-order Couplings

We will discuss recursive numerical integration as an efficient method to compute discretized path integrals in systems with low-order couplings. Low-order couplings arise in many physical systems as a consequence of locality exhibited by the underlying physical model. As such, discretizing space-time in a physical theory with locality implies that any given point of that discretized space-time can only be directly influenced by its nearest neighbors and we will show that recursive numerical integration excels in these situations leading to exponential error scaling.

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MS127

New Efficient High Dimensional Integration Rules for Quantum Field Theoretical Models

We present an investigation of a fully symmetric integration over compact groups in the case of a 0+1 dimensional system and the discretised quantum mechanical model, the topological rotor. While in the case of the 0+1 dimensional model the method works perfect up to arbitrary machine precision, for the quantum mechanical system we were not able to find an improvement over conventional Markov chain Monte Carlo methods. We will give an explanation for this finding and suggest revenues to overcome this failure.

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MS127

Quasi-Monte Carlo Sampling for the Schrödinger Equation

We approximate the solution of the time-dependent Schrödinger equation with a two step procedure. We sample the physical domain using a rank-1 lattice rule and apply Strang splitting for time-stepping. We derive theoretical results which show advantages and advances over previous methods which are also demonstrated by numerical results. This is joint work with Yuya Suzuki and Gowri Suryanarayana.

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MS128

UQTk - A Flexible Python/C++ Toolkit for Uncertainty Quantification

The UQ Toolkit (UQTk) is a collection of libraries, tools and apps for the quantification of uncertainty in numer-

ical model predictions. UQTk offers intrusive and non-intrusive methods for forward uncertainty propagation, tools for sensitivity analysis, sparse surrogate construction, and Bayesian inference. The core libraries are implemented in C++ but a Python interface is available for easy prototyping and incorporation in UQ workflows. We will present the core UQTk design philosophy and illustrate key capabilities.

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MS128

Chaospy: A Pythonic Approach to Polynomial Chaos Expansion

Polynomial chaos expansion is a popular method for extracting statistical metrics from solutions of forward problems with well characterized variability in the model parameters. Chaospy is a Python toolbox specifically developed to implement polynomial chaos expansions using the high modularity and expressiveness of Python. The toolbox allows for implementation of an expansion using only a handful lines of code. More over, Chaospy is a development foundry that allows for easy experimentation with custom features beyond the scope of standard implementation. To demonstrate the capabilities of the Chaospy toolbox, this talk will demonstrate how polynomial chaos expansions can be applied on an intrusive Galerkin problem. Intrusive problem formulation often requires the reformulation and solving of a set of governing equations, and does not conform well to standardized tools. As such, the number of available tools to solve these type of problems are limited.

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MS128

Prediction and Reduction of Runtime in UQ Simulations on HPC Systems using Chaospy

For non-intrusive UQ simulations many black box model evaluations have to be performed. If the runtime of a model is sensitive to the uncertain input parameters, the runtime may vary significantly for each model run. In this talk, we present a novel idea by building a surrogate of the runtime of a model. With this surrogate we can predict and reduce the total runtime of UQ simulations on HPC systems. We examined this with Chaospy.

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MS128

A Standard for Algorithms of Numerical Experiments: Proposal, Implementation and Feedback

The GdR MASCOT-NUM holds exchanges between practitioners and designers of many numerical experiments field: sensitivity analysis, optimisation, inversion, ... As many software platforms are now available for industrial usage, it will become efficient to side this growing usage with some standardisation. Indeed, our critical point stands in the transfer of scientific developments to industrial applications, so the greatest improvement should be awaited from a leaner transfer process. We propose such a preliminary standard for development of numerical experiments (for many common languages), carrying about minmal constraints for implementations, considering that this task is still often considered as optional and costly by designers of such algorithms. We then demonstrate immediate benefits on some basic examples: automated testing, benchmarking and smooth platform integration. We will focus on some support online tools that also widely improve end users advertising and feedback.

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PP1

Modeling Nonstationary Response Surfaces with Bayesian Warped Gaussian Processes

A common challenge in constructing a surrogate model for uncertainty propagation is that the response exhibits nonstationary behavior. A popular method for overcoming this is to decompose the surrogate into many local models via adaptive refinement. However, such models quickly run into difficulties when either the dimensionality of the input space is high or when the nature of the nonstationarity is complicated. In such cases, a nonlocal, nonparametric method seems appropriate. We show how the framework of the Bayesian warped Gaussian process [Lázaro-Gredilla, NIPS 12] can be specially applied to problems in UQ to overcome this issue. In the first GP layer, the stochastic variables parameterizing the uncertain inputs to the simulator are propagated into an intermediate, warped latent space. From here, one appends the spatiotemporal input data from the simulator run data to learn a mapping to the corresponding simulator outputs. Joint training of the two layers ensures that the transformed latent space is amenable to the stationary assumption of the second GP layer, and the nonparametric nature of the layers makes the warping layer effective with complicated nonstationarities. Furthermore, we exploit separability properties in the latent layer yielding a sparse GP model with efficient Kronecker product decompositions, allowing for GP modeling of millions of data. The approach is demonstrated on dynamical ODEs and nonlinear elliptic PDEs with nonstationary features.

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PP1

Bayesian Optimization with Variables Selection

Bayesian optimization techniques have been successfully applied in various fields of engineering. Generally, they are used in the case of a moderate number of variables. Therefore, there is a great interest in Bayesian optimization algorithms suitable for high-dimensional problems. Here, we consider the high-dimensional case with a moderate number of influential variables. The basic idea consists in filtering the minor variables in order to enhance the optimization. To do so, new criteria are introduced within the Gaussian Process regression model and a specific set of stationary kernels. The proposed algorithm combines optimization and variables selection. The points are generated in order to accelerate the optimization and refine the variables selection. The parameters splitting is challenged sequentially thanks to a new criterion called doubt. The algorithm is tested and compared to other methods such as the classical EGO. The results show the efficiency of the algorithm for high dimensional problems when the intrinsic dimensionality is moderate.

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PP1

Bayesian Inference and Statistical Modeling with TransportMaps

TransportMaps is a Python module for the solution of Bayesian inference problems through measure transport and variational methods. The core methodology consists in the creation of a mapping, of adjustable complexity, between a tractable distribution and the intractable distribution of interest. This map can be used directly for the generation of quadrature rules and/or independent samples with respect to the intractable distribution. Alternatively, the map can be used to precondition other Bayesian inference methods, such as Markov chain Monte Carlo. The software provides a number of algorithms built on top of this framework: adaptive construction of transport maps [Bigoni D., et al., *On the computation of monotone transports*], sequential inference using low-dimensional couplings [Spantini, A., et al. (2017), *Inference via low-dimensional couplings*. http://arxiv.org/abs/1703.06131], sparsity identification of non-Gaussian graphical models [Morrison, R., et al. (2017), *Beyond normality: Learning sparse probabilistic graphical models in the non-Gaussian setting*, NIPS 2017], approximate nonlinear filtering [Spantini, A., (2017), in PhD thesis: *On the low dimensional structure of Bayesian inference*]. Additionally the software provides a flexible modeling language for statistical problems, allowing for its integration with existing software. Software and documentation: `http://transportmaps.mit.edu`

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PP1

Simulation-based Machine Learning: An Application to Structural Health Monitoring

The continuous development of computational models and experimental engineering has led to the development of data assimilation methodologies. Among the applications of data assimilation we focus on structural health monitoring, which refers to damage detection strategies applied to aerospace, civil or mechanical engineering. By using a data-based approach we perform risk-based decisions in real time. This approach builds a mathematical model for a digital twin, which is an approximation of the real structure of interest, to create a dataset of all possible healthy states. This synthetic dataset, composed of selected features, is then used to train a classifier, which can assess the state of damage of the structure based on experimental measurements. We explore different machine learning algorithms with a particular focus on a One Class Support Vector Machine to detect anomalies and the Artificial Neural Networks to predict real-valued quantities of interest. The parametric mathematical model is perturbed to include natural variations of some physical and geometrical parameters. The latter are obtained via a pre-computed parameter estimation using a Bayesian approach. Because of the large parameter space a model order reduction strategy is exploited to reduce the computational burden. We apply this strategy to the two-dimensional acoustic-elastic wave equation and show the effectiveness of the method for detecting cracks and monitor the damage state of the system.

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PP1

Efficient Uncertainty Propagation of Physics-based Nondestructive Measurement Simulations using Sparse Sampling and Stochastic Expansions

The practice of determining the probability of defect detection for a nondestructive testing (NDT) inspection through use of computational measurement simulation is recognized for its potential cost savings and improved accuracy. However, measurement simulation covering the full range of possible random input parameters most often represents a prohibitively large computational task, particu-

larly when using time-consuming physics-based numerical simulations. This work presents the application of efficient uncertainty propagation of physics-based NDT simulations using sparse sampling and stochastic expansions. In particular, polynomial chaos expansions (PCE) are used to construct fast surrogate models of the computational simulations and perform the uncertainty propagation. More specifically, three types of PCE models are used, namely, quadrature, ordinary least squares, and least-angle regression sparse. The approach is demonstrated on model-assisted probability of detection of a spherical void defect in a quartz block using ultrasonic testing simulation with a focused transducer and three uncertain input parameters. The results are compared with direct Monte Carlo sampling (MCS), as well as with MCS and deterministic Kriging surrogate models. For this case, the PCE methods show around three orders of magnitude faster convergence on the statistical moments over direct MCS, and needing hundreds of fewer samples than Kriging to reach the same level of modeling accuracy.

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PP1

Sparse Pseudo-spectral Projections in Linear Gyrokinetics

The simulation of micro-turbulence in plasma fusion is paramount for understanding the confinement properties of fusion plasmas with magnetic fields. It is driven by the free energy provided by the unavoidably steep plasma temperature and density gradients. Unfortunately, the measurement of the latter - as well as further decisive physics parameters affecting the underlying micro-instabilities - are subject to uncertainties which requires an uncertainty quantification framework. Here, we employ the established plasma micro-turbulence simulation code GENE (`genecode.org`) and restrict ourselves to the linear gyrokinetic eigenvalue problems in 5D phase space, taking into account electrons and deuterium ions. Even without the nonlinear terms, the computational requirements are enormous and given the large number of uncertain parameters, quantifying uncertainty remains challenging. To overcome these issues, we employ adaptive pseudo-spectral projections constructed on Leja sequences. We test the approach in two test cases, a modified benchmark case, in which we consider two or seven stochastic inputs, and a real world scenario having 11 stochastic inputs. Our results show that sparse pseudo-spectral projections are suitable for overcoming the challenges of quantifying uncertainty in linear gyrokinetics. Furthermore, the total Sobol indices for global sensitivity analysis show that out of all stochastic inputs, the two temperature gradients are the most relevant.

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PP1

Comparing Two Dimension Reduction Techniques

When working with high dimension models, it is often useful to create a surrogate model of lower dimension. With a surrogate model in hand, we may be able to compute Quantities of Interest more efficiently. Two dimension reduction techniques – Principal Component Analysis (PCA) and Active Subspace analysis – will each be used to create a surrogate model which approximates the action of a high-dimension, algebraic model. At their core, PCA and Active Subspace analysis can be roughly described as eigenvalue analysis of a covariance matrix. The example presented is intended highlight the subtle differences, along with the pro's and con's of each approach.

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PP1

Künzel Model and Non-Intrusive Inverse Problem

In specific fields of research such as preservation of historical structures, medical imaging, material science, geophysics and others, it is of particular interest to perform only a non-intrusive boundary measurement. The main idea is to obtain comprehensive information of material properties inside the domain under consideration while maintaining the test sample intact. The forward model is represented by Künzel model with a finite element discretization and parameters are subsequently recovered using a modified Calderón problem principle, numerically solved by a regularized Gauss-Newton method. We provide a basic framework, implementation details and modification of general constrains originally derived for a standard setup of Calderón problem. The proposed model setup is numerically verified for various domains, load conditions and material field distributions.

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PP1

Optimal Kernel-based Dynamic Mode Decomposition

This work focuses on the reduced modeling of a dynamical system based on a finite approximation of the Koopman operator. The reduced-model is obtained by determining the so-called extended dynamic mode decomposition (EDMD). This decomposition characterises the eigen-

structure of the solution of a least square problem subject to low-rank constraints. Because of the too large dimension of the state space, algorithms solving this problem need to rely on kernel-based methods. However, the state-of-the-art kernel-based algorithm known as K-DMD provides a sub-optimal solution to this problem, in the sense it relies on abusive approximations and on many restrictive assumptions. The purpose of this work is to propose an optimal kernel-based algorithm able to solve exactly this low-rank approximation problem in a general setting.

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PP1

Heterogeneous Material Model Calibration using Stochastic Inversion

In order to calibrate a heterogeneous material model from noisy experimental data the corresponding uncertainties have to be taken into account in a proper way. The underlying step is to distinguish aleatory from epistemic uncertainties and treat these two types of uncertainties separately. The goal of the identification process is to quantify the aleatory uncertainties expressing the inherent randomness of heterogeneous material properties while the epistemic uncertainties are reduced with any new measurement. From this perspective, the calibration of a heterogeneous material model is a stochastic inverse problem which can be solved with the help of the Bayesian inference.

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PP1

Bootstrap Stochastic Approximation Monte Carlo Algorithms

Markov chain Monte Carlo (MCMC) simulation methods have been widely used as a standard tool in Bayesian statistics in order to facilitate inference. Nowadays, many real world applications involve large data-sets with complex structures and require complex statistical models to account for these structures. We develop the bootstrap stochastic approximation Monte Carlo algorithm that makes the analysis of big-datasets feasible by avoiding repeated scans of the whole data-sets and mitigates the local trapping problems that MCMC algorithms often encounter. Hence our algorithm is suitable to address problems with both large data-sets and complex statistical models. The performance of the algorithm will be assessed in a simulation study. The algorithm will me implemented to train a surrogate model in a real word problem with Big-data.

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PP1

Slow Scale Split Step Tau Leap Method for Stiff Stochastic Chemical Systems

Tau-leaping is a family of algorithms for the approximate simulation of discrete state continuous time Markov chains. The motivation for the development of such methods can be found, for instance, in the fields of chemical kinetics and systems biology. It is well known that the dynamical behavior of biochemical systems is often intrinsically stiff representing a serious challenge for their numerical approximation. The naive extension of stiff deterministic solvers to stochastic integration usually yields numerical solutions with either impractically large relaxation times or incorrectly resolved covariance. We propose a novel splitting heuristic which allows to resolve these issues. The proposed numerical integrator takes advantage of the special structure of the linear systems with explicitly available equations for the mean and the covariance which we use to calibrate the parameters of the scheme. It is shown that the method is able to reproduce the exact mean and variance of the linear scalar test equation and has very good accuracy for the arbitrarily stiff systems at least in linear case. The numerical examples for both linear and nonlinear systems are also provided and the obtained results confirm the efficiency of the considered splitting approach.

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PP1

Robust Experiment Design for Nonlinear Model Calibration using Polynomial Chaos

Traditional approach to design of experiment for calibration of nonlinear material model uses a linearisation and requires some expert prior guess about the values of identified material properties. Robust variant can be then formulated as a worst case approach, where the linearised criterion is evaluated in a set of feasible values of identified parameters and the maximal value is minimised. In the proposed contribution, the linearisation is replaced by considering nonlinear approximation of the material model using a higher order polynomial chaos expansion. The optimality criterion is then integrated over the feasible domain of material parameters instead of considering a set of their discrete values.

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PP1

Locally Stationary Spatio-Temporal Interpolation of Argo Profiling Float Data

Argo floats measure sea water temperature and salinity in the upper 2,000 m of the global ocean. The statistical analysis of the resulting spatio-temporal dataset is challenging due to its non-stationary structure and large size.

We propose mapping these data using locally stationary Gaussian process regression where covariance parameter estimation and spatio-temporal prediction are carried out in a moving-window fashion. This yields computationally tractable non-stationary anomaly fields without the need to explicitly model the non-stationary covariance structure. We also investigate Student-t distributed microscale variation as a means to account for non-Gaussian heavy tails in Argo data. We use cross-validation to study the point prediction and uncertainty quantification performance of the proposed approach. We demonstrate clear improvements in the point predictions and show that accounting for the non-stationarity and non-Gaussianity is crucial for obtaining well-calibrated uncertainties. The approach also provides data-driven local estimates of the spatial and temporal dependence scales which are of scientific interest in their own right.

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PP1

Solving Stochastic Inverse Problems with Consistent Bayesian Inference

We study a data-oriented (aka consistent) Bayesian approach for inverse problem. Our focus is to investigate the relationship between the data-oriented Bayesian formulation and the standard one for linear inverse problems. We show that 1) from a deterministic point of view, the MAP of the data-oriented Bayesian method is similar to the truncated SVD approach (regularization by truncation), and 2) from the statistical point of view, no matter what prior is used, the method only allows the prior to act on the data uninformed parameter subspace, while leaving the data-informed untouched. Both theoretical and numerical results will be presented to support our approach.

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PP1

Multilevel Adaptive^2 Sparse Grid Stochastic Collocation

Randomness in Uncertainty Quantification problems can often be modeled by using a truncated Karhuenen-Loeve (KL) expansion. This applies for partial differential equations with random coefficients as well as for random ordinary differential equations, which involve random processes. Since the number of terms in the KL expansion directly translates into the number of stochastic dimensions we, however, quickly run into the curse of dimensionality. The most commonly used approach is Monte Carlo, which in general, however, converge slowly. Since the KL modes decrease exponentially, we instead apply adaptive sparse grid surrogates to leverage anisotropy in the solution. To add an additional adaptive layer, we drew inspiration from the multilevel collocation approach which directly relates to the combination technique. Thus, we define two grid layers: on the lower layer, we employ a dimension-adaptive sparse grid to interpolate the output for a given tolerance. On the upper layer, we construct an abstract three-dimensional sparse grid having as dimensions the aforementioned lower layer tolerance, the number of KL terms, and the time step size; finally the solutions are combined using the combination technique on the upper level. This deterministic approach offers solutions with the same accuracy as a single high resolution adaptive sparse grid, however with much lower computational cost by leveraging the nestedness and anisotropy of the underlying problem.

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PP1

Efficient Iterative Methods for Discrete Stokes Equations with Random Viscosity

We study the stochastic Galerkin finite element (SGFE) discretization of Stokes flow with random viscosity and the resulting discrete saddle point problem. In order to deal with the large coupled system of equations efficiently, fast solution methods are essential. In our work, we investigate the performance of different iterative solvers. As the discrete SGFE problem can be arranged in a way that the system of equations is structurally equivalent to the purely spatial one, we rely on iterative solvers designed for discrete Stokes equations with deterministic data. For the preconditioners, we prescribe a Kronecker product structure and use existing approaches from the finite element and stochastic Galerkin literature as building blocks. We derive analytical bounds for the eigenvalues of the preconditioned system matrices and use them to predict the convergence behavior of the iterative solvers. By the help of a numerical test case, we verify the theoretical predictions for a block diagonal preconditioned MINRES method and a block triangular preconditioned Bramble-Pasciak conjugate gradient method. We eventually compare the solvers based on two criteria: the computational complexity of the underlying algorithms and the convergence behavior of the methods with respect to different problem parameters.

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PP1

Optimal Experimental Design of Time Series Data in a Consistent Bayesian Framework

To quantify uncertainties of inputs to models of dynamical systems, a fixed spatial configuration of sensors is often designed and deployed to collect time-series data for solving stochastic inverse problems. A general goal is to configure the sensors so that they provide useful information for the stochastic inverse problem over the full duration of the experiment and provide us with minimally redundant data. We use a recently developed Consistent Bayesian framework for formulating and solving stochastic inverse problems to investigate several design criteria and objectives for deploying sensors. We draw comparisons to other approaches and results based on more classical statistical Bayesian formulations.

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PP1

Quantifying Spatio-temporal Boundary Condition Uncertainty for the Deglaciation

Ice sheet models are currently unable to reproduce the retreat of the North American ice sheet through the last deglaciation, due to the large uncertainty in the boundary conditions. To successfully calibrate such a model, it is important to vary both the input parameters and the boundary conditions. These boundary conditions are derived from global climate model simulations, and hence the biases from the output of these models are carried through to the ice sheet output, restricting the range of ice sheet output that is possible. Due to the expense of running global climate models for the required 21,000 years, there are only a small number of such runs available; hence it is difficult to quantify the boundary condition uncertainty. We develop a methodology for generating a range of plausible boundary conditions, using a low-dimensional basis representation for the spatio-temporal input required. We derive this basis by combining key patterns, extracted from a small climate model ensemble of runs through the deglaciation, with sparse spatio-temporal observations. Varying the coefficients for the chosen basis vectors and ice sheet parameters simultaneously, we run ensembles of the ice sheet model. By emulating the ice sheet output, we history match iteratively and rule out combinations of the ice sheet parameters and boundary condition coefficients that lead to implausible deglaciations, reducing the uncertainty due to the boundary conditions.

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PP1

Multiscale Interfaces for Large-scale Optimization

In this poster we describe MILO (Multiscale Interfaces for Large-scale Optimization), a software package built from components of the Trilinos project that aims to provide a lightweight PDE-constrained optimization solver with a multiscale modeling capability. The use of template-based metaprogramming automatic differentiation allows a user to specify a variety of forward models through a syntax that closely resembles pencil-and-paper variational formulations and automates adjoint computations. State of the art optimization under uncertainty algorithms are available through an interface to the Rapid Optimization Library. Finally, the software contains an implementation of a generalized mortar method for flexible modeling, optimization, and uncertainty quantification of multiscale physical phenomena.

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PP1

A Study of Elliptic PDEs with Jump Diffusion Coefficients

As a simplified model for subsurface flows elliptic equations may be utilized. Insufficient measurements or uncertainty in those are commonly modeled by a random coefficient, which then accounts for the uncertain permeability of a given medium. As an extension of this methodology to flows in heterogeneous\fractured\porous media, we incorporate jumps in the diffusion coefficient. These discontinuities then represent transitions in the media. More precisely, we consider a second order elliptic problem where the random coefficient is given by the sum of a (continuous) Gaussian random field and a (discontinuous) jump part. To estimate moments of the solution to the resulting random partial differential equation, we use a pathwise numerical approximation combined with multilevel Monte Carlo sampling. In order to account for the discontinuities and improve the convergence of the pathwise approximation, the spatial domain is decomposed with respect to the jump positions in each sample, leading to pathdependent grids. Hence, it is not possible to create a nested sequence of grids which is suitable for each sample path a-priori. We address this issue by an adaptive multilevel algorithm, where the discretization on each level is sample-dependent and fulfills given refinement conditions. This is joint work with Andrea Barth (SimTech, University of Stuttgart)

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PP1

Image-based Covariance Functions for Characterisation of Material Heterogeneity

The principal challenge in implementation of random fields arises from the need for determination of their correlation/characteristic lengths in the simplest case or more generally their covariance functions. The present contribution

is devoted to the construction of random fields based on image analysis utilising statistical descriptors, which were developed to describe the different morphology of random material.

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PP1

Numerical Algorithms for Solving the Weighted Poisson Equation with Application to Particle Flow Algorithms

The poster is concerned with numerical algorithms for solving the Poisson equation. The Poisson equation is a partial differential equation that involves a probability weighted Laplacian. The problem is to approximate the solution to the Poisson equation using *only* particles sampled from the probability distribution. The solution of the Poisson equation plays a central role in particle flow algorithms for solving the nonlinear filtering problem. The particle flow algorithms are exact, i.e they exactly represent the posterior distribution, if the Poisson equation is solved exactly. Two algorithms for solving the Poisson equation are presented: a Galerkin algorithm and a kernel-based algorithm. The Galerkin algorithm is based on the projection of the solution to the span of preselected basis functions. The kernel-based algorithm is based on expressing the Poisson equation as a fixed point problem involving the semigroup associated with the weighted Laplacian. The poster contains error analysis of both algorithms. The significant result is that the error of the kernel-based algorithm converges to zero in the asymptotic limit as the number of particles goes to infinity. The result also includes convergence rate. This result is important since it is the first step for error analysis of the particle flow algorithms in the nonlinear setting.

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PP1

Stochastic Galerkin Reduced Basis Methods for Parametrized Elliptic PDEs

We propose stochastic Galerkin reduced basis (RB) methods to estimate statistics of linear outputs in the context of parametrized elliptic PDEs with random data. For a given value of a deterministic parameter vector, a stochastic Galerkin finite element method can estimate output statistics at essentially the cost of a single solution of a very large linear algebraic system of equations. To lower the time and memory requirements, we derive a Galerkin RB method by projecting the parametrized spatial-stochastic weak form of the problem onto a POD subspace. As a consequence, the complexity of the reduced problem becomes essentially independent of the number of stochastic Galerkin finite element degrees of freedom. Statistical moments of the reduced solution can be computed by exact integration. Consequently, they are only subject to an RB approximation error but not subject to quadrature errors like in Monte Carlo sampling or stochastic collocation. Moreover, standard RB theory provides computable a posteriori error bounds for the RB approximation error of parameter-dependent output statistics. We present numerical tests for a diffusion reaction problem, where the reaction coefficient acts as a deterministic parameter and a Karhunen-Loeve decomposed random diffusion field acts as a random input. Compared to a Monte Carlo RB method, statistical estimation with our method is significantly faster, because it requires only a single solution of a reduced system of comparable size.

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PP1

Adaptive Gaussian Process Approximation for Bayesian Inference with Expensive Likelihood Functions

We consider Bayesian inference problems with computationally intensive likelihood functions. We propose a Gaussian process (GP) based method to approximate the joint distribution of the unknown parameters and the data, built upon a recent work. In particular, we write the joint density approximately as a product of an approximate posterior density and an exponentiated GPsurrogate. We then provide an adaptive algorithm to construct such an approximation,w here an active learning method is used to choose the design points. With numerical examples, we illustrate that the proposed method has competitive performance against existing approaches for Bayesian computation.

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PP1

A Comparative Study of the Intrusive and Non-intrusive Polynomial Chaos Methods for Uncertainty Quantification of the Rossler Chaotic Dynamical System

The simulations of dynamical system models contain significant uncertainty, which usually arises from errors initial conditions and model parameters. Uncertainty quantification, thus, is of critical importance in improving system simulations. This work aims to intercompare the effectiveness and efficiency of intrusive and non-intrusive polynomial chaos methods for uncertainty quantification of the non-deterministic simulations of the Rossler chaotic dynamical system. The simulation results are verified and confirmed by comparing the results obtained using the Monte Carlo method. The results show that both of the polynomial chaos methods can effectively simulate the propagation of uncertainties in chaotic dynamical system and are more effective and efficient than the Monte Carlo method. Through the comparative study, the strengths and weaknesses of intrusive and non-intrusive polynomial chaos methods for uncertainty quantification are discussed.

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PP1

A Model-independent Iterative Ensemble Smoother for High-dimensional Inversion and Uncertainty Estimation

We have implemented an iterative Gauss-Levenburg-Marquardt (GLM) form of the ensemble smoother that functions in a model-independent way by programmatically interacting with any forward model. Using the ensemble approximation to the tangent linear operator (Jacobian) allows the GLM algorithm to be applied to extremely high dimensions with manageable computation burden, provides some enhanced non-linear solution capabilities, and also yields uncertainty estimates. The implementation includes the capability for testing multiple lambda values and TCP/IP parallelization. Furthermore, a subset of the entire ensemble can be used to test the lambda values, reducing the number of model evaluations required. An example application from groundwater hydrology is presented. The results of the iterative ensemble smoother are compared to deterministic inversion and to Monte Carlo results.

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PP1

Physics-informed Machine Learning for Data-driven Turbulence Modeling

Reynolds-averaged Navier-Stokes (RANS) models are still workhorse tool in engineering applications that involve turbulent flows. It is well known that the RANS models introduce large model-form uncertainties into the prediction. Recently, data-driven methods have been proposed as a promising alternative by using existing database of experiments or high-fidelity simulations. In this poster, we present a physics-informed machine-learning-assisted turbulence modeling framework. This framework consists of three components: (1) construct a functional mapping between physics-informed inputs and Reynolds stress based on DNS data via machine learning techniques, (2) assessing the prediction confidence a priori by evaluating the distance between different flows in the mean flow features space, and (3) propagating the predicted Reynolds stress field to mean velocity field by using physics-informed stabilization. We evaluate the performance of proposed by using several flows with massive separations. Significant improvements over the baseline RANS simulation are observed for both the Reynolds stress and the mean velocity fields. In addition, the prediction performance based on different training flows can be assessed a priori by using the proposed distance metrics.

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PP1

Calibration Optimal Designs for Computer Experiments

History matching with Gaussian process emulators is a well-known methodology for the calibration of computer models based on partial observations (Craig et al., 1996). History matching is a method that attempts to identify the parts of input parameter space that are likely to result in mismatches between simulator outputs and observations. A measure called implausibility is used to rule out parameter settings that are far from the observations. The space that has not yet been ruled out is called Not Ruled Out Yet (NROY) space. An easily neglected limitation of this method is that the emulator must simulate the target NROY space well, else good parameter choices can be ruled out. We show that even when an emulator validates well on the whole parameter space, good parameter choices can be ruled out in simple test case. If a Bayesian calibration were tried here, the biases in the NROY region would lead to strong biases in the calibration. We present novel methods for detecting these cases and calibration optimal designs for subsequent experiments that ensure the true NROY space is retained and parameter inference is not biased.

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PP101

Visualizing Dynamic Global Sensitivities in Time-dependent Systems

Several problems in uncertainty quantification suffer from the curse of dimensionality. The best way to alleviate the curse is to reduce the dimension. This minisymposterium will explore several ideas for parameter space dimension reduction that enable otherwise infeasible uncertainty quantification studies for computational science models with several input parameters. This poster will explore visualizing how global sensitivities of dynamical systems change over time.

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PP101

Parameter Space Dimension Reduction

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duction that enable otherwise infeasible uncertainty quantification studies for computational science models with several input parameters.

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PP101

A Lanczos-Stieltjes Method for One-dimensional Ridge Function Integration and Approximation

Several problems in uncertainty quantification suffer from the curse of dimensionality. The best way to alleviate the curse is to reduce the dimension. This minisymposterium will explore several ideas for parameter space dimension reduction that enable otherwise infeasible uncertainty quantification studies for computational science models with several input parameters. This poster focuses on an approach to approximating one-dimensional ridge functions based on the Lanczos iteration.

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Characterizing a Subspace of Shapes using Differential Geometry

Engineering designers routinely manipulate the shapes in engineering systems toward design goals—e.g., shape optimization of an airfoil. The computational tools for such manipulation include parameterized geometries such as B-splines, where the parameters provide a set of independent variables that control the geometry. Recent work has developed and exploited *active subspaces* in the map from geometry parameters to design quantities of interest (e.g., lift or drag of an airfoil); the active subspace is a set of directions in the geometry parameter space that changes the associated quantity of interest more, on average over the design space, than directions orthogonal to the active subspace. The active directions produce insight-rich geometry perturbations; however, these perturbations depend on the chosen geometry parameterization. In this work, we use tools and concepts from differential geometry to develop parameterization independent active subspaces with respect to a given scalar field (e.g., the pressure field surrounding an airfoil). The differential geometry setup leads to consistent numerical discretization. We show how the framework can yield insight into the design of an airfoil independent of the choice of parameterization.

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PP101

Exploiting Ridge Structure in Chance Constrained Design under Uncertainty

A chance constrained design problem consists of several quantities of interest defined over a set of design and random variables with the goal of minimizing (for example) the expected value of one quantity of interest subject to the constraint that the probability of the other quantities of interest exceed a threshold is less than a specified probability. In the absence of exploitable structure where we only have access to function samples, this is a challenging problem. Evaluating the probability constraints via Monte-Carlo requires many evaluations of potentially expensive quantities of interest. However, if the chance constraint quantities of interest exhibit ridge structure – that is, these functions only vary with respect to a few linear combinations of the input variables – we can replace these chance constraints with a bound constraint over the design variables. This replacement removes the need evaluate the quantities of interest to ensure the chance constraints are satisfied, substantially decreasing the cost of chance constrained design problems where the quantities of interest involve large scale, complex computational models.

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