Abstracts

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IP1

Prediction, State Estimation, and Uncertainty Quantification for Complex Turbulent Systems

Complex Turbulent Systems such as those in climate science and engineering turbulence are a grand challenge for prediction, state estimation, and uncertainty quantification (UQ). Such turbulent dynamical systems have an erroneous phase space with a large dimension of instability and crucial extreme events with major societal impact. Monte Carlo statistical predictions for complex turbulent dynamical systems are hampered by severe model error due to the curse of small ensemble size with the overwhelming expense of the forecast model and also due to lack of physical understanding. This lecture surveys recent strategies for prediction, state estimation, and UQ for such complex systems and illustrates them on prototype examples. The novel methods include physics contrained nonlinear regression strategies for low order models, calibration strategies for imperfect models combining information theory and statistical response theory, and novel state estimation algorithms.

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IP2

Sparse Grid Methods in Uncertainty Quantification

In this presentation, we give an overview on generalized sparse grid methods for stochastic and parametric partial differential equations as they arise in various forms in uncertainty quantification. We focus on the efficient approximation and treatment of the stochastic/parametric variables and discuss both, the case of finite and infinite/parametric stochastic dimension. Moreover, we deal with optimal numerical schemes based on sparse grids where also the product between the spatial and temporal variables and the stochastic/parametric variables is collectively taken into account. Overall, we obtain approximation schemes which involve cost complexities that resemble just the cost of the numerical solution of a constant number of plain partial differential equations in space (and time), i.e. without any stochastic/parametric variable. Here, this constant number depends only on the covariance decay of the stochastic fields of the input data of the overall problem.

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IP3

Covariance Functions for Space-time Processes and Computer Experiments: Some Commonalities and Some Differences

Gaussian processes are commonly used to model both natural processes, for which the indices are space and/or time, and computer experiments, for which the indices are often parameters of the computer model. In both settings, the modeling of the covariance function of the process is critical. I will review various approaches to modeling covariance functions for natural processes, with a focus on the space-time setting. I will then consider what lessons, if any, can be drawn from this work for modeling covariance functions for computer experiments.

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IP4

Reduction of Epistemic Uncertainty in Multifidelity Simulation-Based Multidisciplinary Design

Epistemic model uncertainty is a significant source of uncertainty that affects the prediction of a multidisciplinary system using multifidelity analyses. Uncertainty reduction can be achieved by gathering additional experiments and simulations data; however resource allocation for multidisciplinary design optimization (MDO) and analysis remains a challenging task due to the complex structure of a multidisciplinary system and the dynamic nature of decision making. We will present a novel approach that integrates multidisciplinary uncertainty analysis (MUA) and multidisciplinary statistical sensitivity analysis (MSSA) to answer the questions about where (sampling locations), what (disciplinary responses), and which (simulations versus experiments) for allocating more resources. The proposed approach strategically breaks resource allocation into a sequential process, the decision making is hence much more tractable. Meanwhile the method is efficient for complex multidisciplinary analysis by employing inexpensive Spatial Random Process (SRP) emulators and analytical formulas of MUA and MSSA.

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IP5

Multi-fidelity Approaches to UQ for PDEs

We discuss the use of a set of multi-fidelity computational physical models for reducing the costs of obtaining statistical information about PDE outputs of interest. Multilevel Monte Carlo and multilevel stochastic collocation methods use a hierarchy of successively coarser discretizations, in physical space, of the parent method. Reduced-order models of different dimension can be also be used as can surrogates built from data. More generally, a management strategy for the use of combinations of these and other computational models is discussed.

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IP6

Uncertainty Quantification in Weather Forecasting

A major desire of all humankind is to make predictions for an uncertain future. Clearly then, forecasts ought to be probabilistic in nature, taking the form of probability distributions over future quantities or events. Over the past decades, the meteorological community has been taking massive steps in a reorientation towards probabilistic weather forecasts, serving to quantify the uncertainty in the predictions. This is typically done by using a numerical model, perturbing the inputs to the model (initial conditions, physics parameters) in suitable ways, and running the model for each perturbed set of inputs. The result is then viewed as an ensemble of forecasts. However, forecast ensembles typically are biased and uncalibrated. These shortcomings can be addressed by statistical postprocessing, using methods such as distributional regression and Bayesian model averaging.

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IP7

Uncertainty Quantification and Numerical Analysis: Interactions and Synergies

The computational costs of uncertainty quantification can be challenging, in particular when the problems are large or real time solutions are needed. Numerical methods appropriately modified can turn into powerful and efficient tools for uncertainty quantification. Conversely, state-of-the-art numerical algorithms reinterpreted from the perspective of uncertainty quantification can becomes much more powerful. This presentation will highlight the natural connections between numerical analysis and uncertainty quantification and illustrate the advantages of re-framing classical numerical analysis in a probabilistic setting. In particular, we will show that using preconditioning as a vehicle for coupling hierarchical models with iterative linear solvers becomes a means not only to assess the reliability of the solutions, but also to achieve super-resolution, as illustrated with an application to magneto-encephalography.

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IP8

Multilevel Monte Carlo Methods

Monte Carlo methods are a standard approach for the estimation of the expected value of functions of random input parameters. However, to achieve improved accuracy often requires more expensive sampling (such as a finer timestep discretisation of a stochastic differential equation) in addition to more samples. Multilevel Monte Carlo methods aim to avoid this by combining simulations with different levels of accuracy. In the best cases, the average cost of each sample is independent of the overall target accuracy, leading to very large computational savings. This lecture will introduce the key ideas, and survey the progress in the area.

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CP1

An Adaptive Algorithm for Stochastic Optimal Control Problems based on Intrusive Polynomial Chaos

We develop an adaptive optimization scheme for uncertain optimal control problems constrained by nonlinear ODEs or differential algebraic equations. The algorithm solves the deterministic surrogate obtained from the intrusive polynomial chaos method by an SQP-based direct optimal control method while simultaneously refining the approximation order using suitable error estimates. The goal is to obtain sufficiently precise estimates of complex quantities such as higher moments while keeping the computational burden feasible for optimal control problems.

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CP1

Uncertainty Quantification of High-Dimensional Stochastic Systems Using Two-Level Domain Decomposition Algorithms

The scalablilities of intrusive polynomial chaos expansion based two-level domain decomposition (DD) algorithms for SPDEs are demonstrated by Subber (PhD thesis, Carleton University (CU), 2012) for high resolution finite element (FE) meshes in the cases of a few random variables. These DD algorithms will be extended here to concurrently handle both high resolution FE meshes and a large number of random variables using the codes developed by the authors.

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CP1

On Efficient Construction of Stochastic Moment Matrices

We consider the construction of stochastic moment matrices that appear in the model elliptic diffusion problem considered in the setting of stochastic Galerkin finite element method (sGFEM). Algorithms for the efficient construction of the stochastic moment matrices are presented for certain combinations of affine/non-affine diffusion coefficients and multivariate polynomial spaces. We report the performance of various standard polynomial spaces for three different non-affine diffusion coefficients in a one-dimensional spatial setting.

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CP1

Iterative Solution of Random Eigenvalue Problem in An Ssfem Framework

This work is aimed at reducing the computational cost of solving the random eigenvalue problem in the weak formulation of spectral stochastic finite element method. This formulation leads to a system of deterministic nonlinear equations, solved using the Newton-Raphson method. The main contribution lies in developing a set of scalable preconditioners for accelerating the computation in a parallel matrix-free implementation. A detailed numerical study is conducted for testing the accuracy and efficiency.

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CP2

Selection and Validation of Models of Tumor Growth in the Presence of Uncertainty

In recent years, advances have been made in the development of multiscale models of tumor growth. Of overriding importance is the predictive power of these models, particularly in the presence of uncertainties. This presentation describes new adaptive algorithms for model selection and model validation embodied in the Occam Plausibility Algorithm (OPAL), that brings together model calibration, determination of sensitivities of outputs to parameter variances, and calculation of model plausibilities for model selection.

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CP2

Dna Pattern Recognition Using Canonical Correlation Analysis

The canonical correlation analysis (CCA) is used as an unsupervised statistical tool to identify patterns. We consider two different semantic objects of DNA sequences as training and test set. CCA check whether the correlation at the point of interest is well above the correlations found elsewhere. As a case study, CCA is applied to investigate HIV-1 preferred integration sites, where the left and right flanking from the integration site are taken as the two views.

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CP2

Modeling the Expected Time to Reach the Recognition Element in Nanopore Dna Sequencing

We examine the functionality of a new approach to next-generation DNA sequencing, where single nucleobases of a DNA oligomer are captured and identified in a modified alpha-hemolysin nanopore. The main uncertainty is when the isolated nucleobases reach a certain location inside the nanopore. We present our model equations and numerical results based on the self-consistent drift-diffusion-Stokes-Poisson system, directed Brownian motion, and a stochastic exit-time problem.

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CP2

Statistical Assessment and Calibration of Ecg Models

We address the problem of calibrating some functional output of a parametrised numerical model to a dataset of real, high dimensional observations. We propose a novel method aiming at reproducing targeted quantiles of the reference data by minimising a suitable probabilistic cost functional defining their statistical spatial quantiles. We apply it to the calibration of models for the simulation of human ECGs (ODE and PDE based) through a dataset of real functional traces.

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CP3

Simplification of Uncertain System to Their Approximate Model

Mathematical modeling of physically available modules result in higher order system, sometime with the uncertainty within, making their study and analysis difficult. Solution to this exists, model order reduction. An effective procedure to obtain a reduced model for an uncertain system using Routh approximant is discussed in this paper. The proposed methodology is an extension of an existing technique for continuous-time domain to discrete-time domain. The algorithm is justified and strengthened by various available examples from the literature.

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CP3

Comparison of Surrogate-Based Uncertainty Quantification Methods for Computationally Expensive Simulators

Polynomial chaos (PC) and Gaussian process (GP) emulation are popular surrogate modelling techniques, developed independently over the last 25 years. Despite tackling similar problems in the field, there has been little comparison of the two methods in the literature. In this work, we build PC and GP surrogates for two black-box simulators used in industry. We assess their comparative performance with changes in design size and type using a number of validation metrics.

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CP3

Randomized Cross Validation

We propose a new randomized cross validation (CV) criterion offering improved performance for model choice in regression problems when the design is not space filling. The proposed criterion is of special interest in environmental and biomedical observation, where strong constraints on placement of measuring points are enforced. The paper presents the new criterion, and demonstrates its superiority with respect to usual CV techniques, considering several alternative regression models as well as simulated and realistic data.

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CP5

Uncertainty Quantification and Sensitivity Analysis for Functional System Response, with An Application to Flyer Plate Experiments

We are usually interested in the functional system response when investigating the shock ignition of explosives. The variation in functional response involves both phase and amplitude, and confounding these two may lead to some problems. In this paper, we derive that the total uncertainty is the sum of the phase and amplitude uncertainty, and give the sensitivity analysis based on this decomposition. Then we apply our method to numerical simulations of a flyer plate experiment.

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CP5

Sobol' Indices for Problems Defined in Non-Rectangular Domains

Uncertainty and sensitivity analysis has been recognized as an essential part of model applications. Global sensitivity analysis based on Sobol' sensitivity indices (SI) offers a comprehensive approach to model analysis by quantifying the relative importance of each input parameter in determining the value of model output. We have developed a novel method for the estimation of Sobol' SI for models in which inputs are confined to a non-rectangular domain (e.g., in the presence of constraints).

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CP5

Sensitivity Analysis with Dependence Measures for Spatio-Temporal Numerical Simulators

The numerical simulators used in environmental applications often deal with complex output parameters such as spatio-temporal, take several uncertain parameters as inputs and can be time expensive. To perform the global sensitivity analysis of such simulators, we propose to use new dependence measures (HSIC) based on reproducing kernel Hilbert spaces. Spatio-temporal HSIC indices and their aggregated versions are thus obtained, yielding the global and local influence of each input variable and its evolution over time.

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CP6

Multidimensional Time Model for Probability Cumulative Function

The new method is based on changes of Cumulative Distribution Function in relation to time change in sampling patterns. Multidimensional Time Model for Probability Cumulative Function can be reduced to finite-dimensional time model with two ordinal numbers 4 for the summation and multiplication over events and their probabilities and ordinal number 17 for the fractal-dimensional time arising from alike supersymmetrical properties of probability.

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CP6

A Bayesian Inference and Importance Sampling Approach to Propagation of Uncertain Probability Distributions

Bayesian inference is used to quantify the uncertainty associated with a distribution derived from data. Yet, in the almost universal case of lack of complete data, the derived distribution cannot be precisely specified. We propose a novel approach, based on Importance Sampling, for propagating uncertain probability distributions. The method identifies an optimal sampling distribution that is representative of the possible range of distributions and adaptively reweights the samples to simultaneously propagate the full range.

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CP7

Some a Priori Error Estimates of Stochastic Galerkin Approximations for Randomly Parameterized ODEs

In this work we focus on generalized polynomial chaos (gPC) based stochastic Galerkin approximations of random ODEs. We provide a priori error estimates for gPC approximations of different classes of first- and second-order random ODEs assuming stochastic regularity conditions for the exact solution. The upper bounds are provided in terms of truncation errors and temporal discretization errors corresponding to different time-stepping schemes. Numerical studies are provided to illustrate some of the theoretical results.

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CP7

Generalised Anova for the Solution of Stochastic Partial Differential Equations

This paper presents a novel approach for the solution of stochastic partial differential equations (SPDE). The proposed approach couples Galerkin projection into the framework of polynomial correlated function expansion, which is the generalisation of the ANOVA decomposition. The framework presented decouples the SPDE into a set of PDEs. The coupled set of PDEs obtained are solved using finite difference method and homotopy algorithm. Performance of the proposed approach has been illustrated with two PDEs.

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CP7

Propagation of Uncertainties for Hyperbolic Equations

Modeling uncertainty propagation in hyperbolic equations and kinetic equations is extremely demanding in terms of robustness and preservation of the maximum properties. This presentation will review new families of such systems with proved BV bounds and maximum preserving estimates. The design of these new systems of PDEs shows connection with L1 minimization techniques and optimal control of polynomial systems.

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CP7

Level Set Methods for Polynomial Chaos Expansion of Stochastic PDEs Outputs

We propose a new method to approximate stochastic solutions of uncertain PDEs using Polynomial Chaos expansions of their level sets. The method is non-intrusive and targets solutions with steep gradients with random locations. An adaptive choice of the level set is used to control the approximation error, ensuring high accuracy at a significantly lower cost compared to classical non-intrusive projection approach. We apply and validate the method on subsurface flows exhibiting steep fronts.

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CP8

Bayesian Parameter Inference with Stochastic Differential Equation Models

Inferring parametric uncertainty, for stochastic differential equation (SDE) models, is a computationally hard problem due to the high dimensional integrals that have to be calculated. Here, we consider the generic problem of calibrating a one dimensional (1D) SDE model to time series and quantifying the ensuing parametric uncertainty. We re-interpret this problem as the problem of simulating the dynamics of a 1D statistical mechanical system and employ a Hamiltonian Monte Carlo algorithm together with multiple time scale integration to solve it efficiently. A generic re-parametrization allows us to solve the dynamics of the fast modes in between measurement points analytically.

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CP8

Residuals in Inverse Problems and Model Form Uncertainty Quantification

Mathematical models often differ in their predictions from experimental observations. Residual errors between a best-fit model and experimental data can be used to investigate missing dynamics. One of the challenges in analyzing residuals is separating deterministic mismatch from variability. We consider in this talk a Bayesian framework for covariance modeling of residuals, an approach that can lead to improved understanding of the uncertainty in model predictions. We illustrate these techniques on a vibration control example.

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CP8

Shape-Constrained Uncertainty Quantification in Unfolding Elementary Particle Spectra at the Large Hadron Collider

The particle spectrum unfolding problem is a statistical inverse problem central to making inferences at the Large Hadron Collider at CERN. Existing methods for constructing confidence intervals in this application can have markedly lower coverage than expected, even for realistic spectra. We present a novel approach that guarantees conservative finite-sample coverage, but still produces usefully tight confidence bounds by imposing physically motivated shape constraints on the particle spectrum using convex optimization.

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CP8

Empirical Evolution Equations

Evolution equations are differential equations that describe the evolution of a system depending on a continuous time variable t. The equation takes the form

$$\dot{\gamma} = v(\gamma)$$

where $\gamma(t) \in X$ is the state of the system at time t, the dot denotes a time derivative, and v is a vector field on X. The space X represents the state space of the system. When X is finite dimensional, the evolution equation reduces to a system of ordinary differential equations. When X is infinite dimensional, the equation can be regarded as a partial differential equation. The classical treatment of evolution equations supposes the vector field v is known and concerns issues including the existence and uniqueness of solutions, the stability of solutions, and the asymptotic behavior of solutions as $t \to \infty$. In this paper we bring a statistical perspective to the study of evolution equations. Our primary curiousity is in performing statistical inference for the solution of the evolution equation when v is estimated, based on a sample of data, by its empirical version $\hat{v}_n$.

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CP9

Quantifying the Degradation in Thermally Treated Ceramic Matrix Composites

Reflectance spectroscopy obtained from ceramic matrix composite is used to quantity the products of oxidation. The data collection will be described in detail in order to point out the potential biasing present in the data processing. A probability distribution is imposed on select model parameters, and then non-parametrically estimated and a pointwise asymptotic confidence band is constructed. An increase in the SiO_2 present was detected in samples as the length of heating was increased.

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CP9

A Bayesian Inversion Approach to Controlled-Source Electromagnetic Imaging

In the Bayesian approach to controlled-source electromagnetic imaging, the objective is to infer the conductivity random field based on finite, noisy measurements of the electromagnetic field. We present a methodology to solve the pertinent non-linear, high-dimensional Bayesian inverse problem by addressing the numerical solution of the parametric, deterministic Maxwell's equations in combination with adaptive sparse-grid interpolation and model order reduction.

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CP9

Spatial Prediction for Quantification of Radar Cross Section Measurement Uncertainty

Uncertainty quantification is an important issue in Radar Cross Section (RCS) measurement, which quantifies the scattering power of an object. At high frequency, the positioning error is a dominant source, difficult to introduce in the uncertainty budget. In our original approach, we show that the RCS uncertainty quantification actually leads to a spatial statistics problem, involving kriging or other spatial prediction methods. The key point is then the prior probabilistic knowledge of the RCS variability.

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CP9

Characterizing Uncertainties in Photoacoustic Tomography

For inverse problems in photoacoustic tomography (PAT), some coefficients of the PDE model must be assumed known in order to perform the reconstruction of other PDE coefficients of greater interest. As these fixed parameters can only be known up to a certain accuracy in practice, this introduces error in the reconstructed images. In this work we quantify the errors in the reconstructed optical parameters of interest caused by model uncertainties in PAT and fluorescence PAT.

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CP10

Performance Tuning of Next-Generation Sequencing Assembly Via Gaussian Process Model with Branching and Nested Factors

For next-generation sequencing data, the selection of assembly tools and the corresponding parameters has a great impact on the quality of de novo assembly. Among assembly tools, there are some shared factors, and some factors are specific to particular tools. Due to complex structures, a tuning procedure is proposed based on the Gaussian process model with branching and nested factors. The performance of the proposed procedure is demonstrated via numerical experiments and a real example.

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CP10

Attitude Determination and Uncertainty Analysis in Eclipse of Small Leo Satellites

Attitude determination concept and uncertainty analysis for LEO hypothetical small satellite with specific emphasis on the eclipse operation are presented. Sensor configurations are used in single-frame method. Common sensors for nanosatellites are selected in order to analyze the uncertainty in the sense of covariance results. For this purpose, covariance and RMS errors with respect to the actual values are presented. In/out of the eclipse period, changing configurations provide better attitude estimation results to filtering techniques.

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CP10

Quantifying Sources of Variability in Planing Hull Experiments

We will present a methodological framework to appropriately handle experimental time history data collected across different study conditions, e.g. variable speeds, size of hull, instrumentation, and facility. We propose a modeling approach that allows for quantification of the different sources of variability inherent to these types of experiments. The experiments relate to an effort to resolve the discrepancy between experimental measurements and simulation-based predictions for planing boats traveling at target speeds through calm water.

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CP10

Study of Detonation Computer Model Calibration with Approximate Bayesian Computing

This paper considers a flyer plate experiment driving by detonation. In this experiment the velocity of free surface was measured. Numerical simulation of the experiment was done by a computer code. In order to determine the parameter of computer model including JWL EOS's parameters, approximate Bayesian computing is used. And then according the post PDF of these parameters, this paper studies the uncertainty quantification of the computer model.

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CP11

Stochastic Modeling of Dopant Atoms in Nanoscale Transistors Using Multi-Level Monte Carlo

We consider the system of stochastic drift-diffusion-Poisson equations to model nanoscale devices such as FinFETs and nanowire sensors. We developed a multi-level Monte-Carlo finite-element method to obtain the current-voltage characteristics as functions of the inherently random doping concentrations. Permittivity, mobility, and forcing terms are random. Finally, we discuss the effect of random-dopant fluctuations on transistor performance, which is the main limiting factor in today's semiconductor technology.

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CP11

Non-Intrusive Stochastic Galerkin Method for the Stochastic Nonlinear Poisson-Boltzmann Equation

The stochastic nonlinear Poisson-Boltzmann equation describes the electrostatic potential in the presence of free charges and has applications in many fields. Here we present a non-intrusive Galerkin method for this nonlinear model equation. It is non-intrusive in the sense that solvers and preconditioners for the deterministic equation can be used as they are. By comparing the non-intrusive stochastic Galerkin method and a stochastic collocation method, it is found that the Galerkin method is a viable option with comparable computational effort.

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CP11

Optimal Method for Calculating Solutions of the Stochastic Drift-Diffusion-Poisson System

The stochastic drift-diffusion-Poisson system has been of great importance for the development of efficient uncertainty-quantification tools for charge transport. We present a rigorous work-and-error analysis of a multi-level estimator for this problem with random permittivities and random forcing terms. We optimize the number of Monte-Carlo samples and the fineness of the mesh in the finite-element method to find the most efficient method to solve this problem. Numerical results support this claim.

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CP12

A Low Rank Kriging for Large Spatial Data Sets

Providing a **b**est **l**inear **u**nbiased **e**stimator (BLUP) is always a challenge for a non-repetitive, irregularly spaced, spatial data. The estimation process as well as spatial prediction involves inverting an $n \times n$ covariance matrix of which typically require computation time of order n^3. Studies showed that often times the complete covariance matrix, can be additively decomposed into two matrices: one from the measurement error modeled as white noise, and the other due to the observed process which can be nonstationary. If nonstationarity is needed, is often assumed to be low rank. Method of **f**ixed **r**ank **k**riging (FRK) developed in Cressie and Johannesson (2008), where the benefit of smaller rank has been used to improve the computation time of order nr^2 where r is the rank of nonstationary covariance matrix. In this work, we consider cholesky decomposition for FRK and use a group-wise penalized likelihood where each row of the lower triangular matrix is penalized. More precisely, we present a two-step approach using group LASSO type shrinkage estimation technique for estimating the rank of the covariance matrix and finally the matrix itself. We implement the block coordinate decent algorithm to obtain the local optimizer to our likelihood problem. We investigate our findings over a set of simulation study and finally apply to a rainfall data obtained on Colorado, US.

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CP12

The "Spatial Boxplot": a Comprehensive Exploratory Tool for Spatial Data

We introduce a versatile exploratory tool that may be used to describe and visualize various distributional characteristics for data with complex spatial dependencies. We present a flexible mathematical framework for modeling spatial random fields, give possible extensions to space-time data, and show mapping hot zones of batting ability in baseball as an illustration.

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CP12

Using Stochastic Estimation for Selective Inversion of Sparse Matrices

The computation of the trace of inverse matrices is a common problem in several applications, from risk analysis to reservoir characterization, requiring the use of selective inversion techniques.In the field of Uncertainty Quantification, both the estimation of the diagonal via unbiased stochastic estimators and the inverse covariance approximation are suitable approaches to this problem. The two methods can be combined in order to obtain an efficient selective inversion framework, with good potential for scaling.

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CP12

The Utility of Quantile Regression in Large Scale Disaster Research

Following disaster, population-based screening programs are routinely established to assess physical and psychological consequences of exposure. These datasets are highly skewed as only a small percentage of trauma-exposed individuals develop health issues. We evaluate the utility of quantile regression in disaster research in contrast to the commonly used population-averaged models with focus on the distribution of risk factors for posttraumatic stress symptoms across quantiles.

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CP13

Estimating Uncertainty in Computer Vision Algorithms

We introduce a statistical framework for estimating the uncertainty given by standard algorithms in computer vision for segmenting an image, by generating realizations of an actual image, which is taken to represent a sample from some distribution of possible observable images. With estimates of segmentation uncertainty for a given image and algorithm, uncertainty can be propagated to measures of an images characteristics. We show the application to quantitative analysis of materials in scanning electron micrographs.

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CP13

Estimation of the Super-Quantile for Optimization - Application in Thermal Engineering

Lifetime's improvement of an electronic component for thermal design can be performed by minimizing a quantile. It is well known that the super-quantile of a distribution is a much more robust quantity. Nevertheless, its estimation can be too costly and the optimization framework implies that this estimation has to be realized on many different samples. In this work, we introduce an efficient estimation of the super-quantile based on a scalar minimization problem and an importance sampling method that allows the use of such minimization. This technique is applied on a thermal use case coming from the TOICA European project (Thermal Overall Integrated Conception of Aircraft).

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CP13

Surrogate Based Inference of Atomic Diffusivity in Metallic Multilayers

The atomic diffusivity in reactive multilayers is characterized by two Arrhenius branches, above and below the melting point of one of its constituents. Observations of homogeneous ignition and of self-propagating fronts are used to infer the corresponding parameters. Posterior distributions are inferred using polynomial chaos surrogates of the observables. Results reveal a large sensitivity to the activation energy and highly correlated posteriors. The potential use of PC surrogates in optimal experimental design is also illustrated.

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CP14

Uncertainty Quantification Approaches for River Hydraulics Modelling

We compare different computational approaches for uncertainty quantification via Monte Carlo and Quasi Monte Carlo simulation in fixed bed river hydraulics modelling.

We assess the sensitivity of the model results with respect to different model parameters and boundary conditions and we study empirically statistical convergence of the output pdfs. Accurate and efficient semi-implicit models are also proposed, that allow to reduce the computational cost of probabilistic open channel flow simulations.

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CP14

Probabilistic Model Identification for the Simulation of Turbulent Flow over Porous Media

In this contribution the application of porous material on the trailing edge of an airfoil for noise reduction is concerned. Herein the focus is on identifying coefficients of a model that simulates the turbulent flow over the porous media by solving the inverse problem in a probabilistic setting. The coefficients of the volume and Reynolds averaged Navier-Stokes equations are modeled as random variables with distributions defined by prior expert knowledge, an then improved by inferring from DNS data of the velocity field and the Reynold stresses.

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CP14

Drop Spreading with Random Viscosity

Motivated by an application in respiratory mechanics, we examine the spreading of a viscous drop over a film, assuming the liquids viscosity is regulated by the concentration of a solute with an initially heterogeneous distribution with prescribed statistical features. We asymptotically reduce the governing nonlinear PDEs to a set of ODEs, allowing stochastic effects to be examined efficiently. In some instances, the variability in the drop's spreading rate can be understood in terms of the spatial sampling of the solute field when the drop is initially deposited on the film.

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CP14

Calibration of a Set of Wall Functions for Turbulent Flows

Wall functions have a significant importance for analysis and simulation of wall-bounded turbulent flows. However, contrary to general belief, their model parameters appear not to be universal. In the present study these parameters are estimated using UQ-techniques applied to publically available numerical and experimental datasets for the canonical flows. Furthermore, an algorithm consisting of a one-dimensional ODE is presented to estimate mean quantities of turbulent channel flow using the resulting wall functions. Sensitivity analysis of this model with respect to various parameters is also addressed.

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CP15

Total Error: Propagation and Partitioning in a Lidar Driven Forest Growth Simulator

The US Forest Service FVS (Forest Vegetation Simulator) is a very widely used growth model developed for projecting individual trees and forest development through time. FVS is now being used to evaluate a variety of global change scenarios as it relates to forest health, carbon life cycle analysis, sustainability, wildlife habitat, wildland fires, etc. In this paper, the total error in form of an uncertainty budget is developed for FVS projections, where initial models inputs are spatially explicit single-tree stem maps developed with small-footprint airborne lidar (Laser Imaging Detection and Ranging). An uncertainty budget shows the overall precision of estimates/predictions made with a system, partitioned according to different types of uncertainty sources within and outside of the system. In a comprehensive fashion, sources of uncertainties due to measurements, classification, sampling error, model parameter estimates, are accounted for in the lidar derived stem maps and within the FVS system. Spatially identifying the sources of uncertainties in time, modeling their propagation and accumulation, and finally, quantifying them locally on a tree basis and globally on a forest level are presented. Uncertainties in future forest responses due to uncertainties in projected global climatic change predictions that will also drive this type of forest model will also be discussed.

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CP15

Uncertainty Propagation Through Multidisciplinary Black-Box Co-Simulation Systems

Modern multidisciplinary sytems (*systems of systems*, e.g. future energy grids) are too complex to be modelled by a small number of people. Instead, component models developed in different institutes may be coupled in a modular manner (*co-simulation*). Due to imperfect knowledge of these component models, they have to be treated as black boxes. We present a modular, non-intrusive, ensemble-based uncertainty quantification framework for *Smart Grid* co-simulation systems considering epistemic as well as aleatory uncertainty.

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MS1

Askit: An Efficient Algorithm for Approximating Large Kernel Matrices

Kernel-based methods are a powerful tool in many inference and learning problems. A key bottleneck in these methods is computations involving the Gram matrix of all pairwise kernel interactions. We describe ASKIT, a scalable, kernel-independent method for approximately evaluating kernel matrix-vector products. ASKIT generalizes the Fast Multipole Method to high-dimensional problems and is based on a randomized method for efficiently factoring off-diagonal blocks. We describe the method and give results on accuracy and scalability.

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MS1

Fast Algorithms for Generating Realisations from High Dimensional Distributions

Generating realisations from high dimensional distributions is computationally expensive, typically scaling as $O(N^3)$, where N is the number of dimensions. The talk discusses a fast direct way of generating realisations from such high dimensional distributions whose complexity scales almost linearly in finite arithmetic.

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MS1

Kernel Methods for Large Scale Data Analysis

In this talk, we focus on kernel techniques for applications in data analysis. The first major step in a practical application is concerned with the modeling. Usually, there is some prior knowledge (such as distances) on the data which needs to be reflected in the reproducing kernel Hilbert space in order to yield a problem-adapted reconstruction scheme. We present a general framework which allows the systematic construction of such smoothness spaces. A technical difficulty which can arise in this procedure is that the kernel itself needs to be numerically computed and hence this numerical error has to be taken care of. To this end, we will give a priori error bounds for the reconstruction error using such manually designed kernels. The second step is on a computational level. Usually in kernel-based methods, one faces large and densely populated ill-conditioned matrices. It is a common observation that some of these numerical problems are due to the chosen basis representation. We will report on recent works to handle the computational issues by problem adapted basis representations. This is partly based on joint work with M. Griebel, B. Zwicknagl (both Bonn University and Peter Zaspel (Heidelberg University).

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MS1

A Robust Parallel Direct Inverse Approximation for Kernel Machine with Applications

We present a parallel direct approximation for fast kernel machine inversion in high dimension, a common problem in data analysis and computational statistics. Fast kernel machine inversion can be viewed as approximation schemes for dense kernel matrix inversion that exploits the hierarchical low-rank structure of the matrix with the help of spatial data structures, typically trees. We introduce a novel parallel inverse approximation for the ASKIT matrix, derive complexity estimates, and apply it to the kernel classification problem.

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MS2

Accelerating the Calibration of High-Resolution Climate Models

Climate models contain numerous parameters associated with aerosols, clouds, and other small-scale physical phenomena. The parameter values are a function of model resolution and must be adjusted for each resolution under consideration. Objective methods for parameter estimation are computationally prohibitive at high resolutions, but can be accelerated by leveraging low resolution simulations that approximate high resolution responses. We illustrate calibration acceleration using a statistical framework that blends climate model ensembles at multiple resolutions. Prepared by LLNL under Contract DE-AC52-

07NA27344.

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MS2

Towards Uncertainty Quantification in 21st Century Sea-Level Rise Predictions: PDE Constrained Optimization as a First Step for Accelerating Forward Propagation

As a first step to quantify the uncertainty of sea level rise predictions due to uncertainty on basal friction coefficient of Greenland ice sheet, we invert for the basal friction field by solving a large-scale PDE constrained optimization problem, minimizing the mismatch with the observations. Then, with the reduced Hessian we compute an approximate Gaussian distribution for the basal friction field, to be used as prior for Bayesian calibration or sampled for Uncertainty Propagation.

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MS2

Quantifying the Impacts of Parametric Uncertainty on Biogeochemistry in the ACME Land Model

Large uncertainties remain in climate predictions, many of which originate from uncertainties in land-surface processes. In particular, uncertainties in land-atmosphere fluxes of carbon dioxide and energy are driven by incomplete knowledge about model parameters and their variation over space and time. Using the ACME land model, we perform uncertainty decomposition based on global Polynomial Chaos (PC) surrogate construction, using the Bayesian Compressive Sensing (BCS) sparse learning technique.

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MS2

Towards Uncertainty Quantification in 21st Century Sea-Level Rise Predictions: Efficient Methods for Forward Propagation of Uncertainty Through Land-Ice Models

This talk will present the evolution of our approach for quantifying uncertainty in anticipated sea-level rise due to melting of the polar ice-sheets. Specifically we will discuss approaches for propagating an uncertain spatially distributed basal friction through a transient ice-sheet model. The run time and high-dimensionality of the transient model pose numerous challenges to most UQ methods. In this talk we will present an initial study that highlights these challenges and discuss avenues for improvement.

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MS3

Hyperbolic Stochastic Galerkin Methods for Nonlinear Systems of Hyperbolic Conservation Laws

When applying the generalized polynomial chaos based stochastic Galerkin method (gPC-SG) to nonlinear systems of hyperbolic conservation laws it generates a system which is not necessarily hyperbolic. In this talk we will introduce a general framework which will avoid this difficulty. We will discuss the general idea, its applications of the compressible Euler and shallow-water equations, and open questions and challenges.

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MS3

MLMC Methods for Computing Measure Valued and Statistical Solutions of Systems of Conservation Laws

We briefly review the theory of entropy measure valued solutions(EMVS), and show how we can compute statistics of multi-dimensional systems of conservation laws using entropy preserving schemes and stochastic sampling. The numerical framework can be improved by Multi-level Monte-Carlo (MLMC) approximations, obtaining a speedup compared to ordinary Monte-Carlo sampling procedure, even in the setting where we do not have convergence of single samples. We also investigate the use computation of statistical solutions to EMVS.

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MS3

Robust Boundary Conditions for Stochastic Incompletely Parabolic and Hyperbolic Systems of Equations

We study hyperbolic and incompletely parabolic systems in three space dimensions with stochastic boundary and initial data. The goal is to show how the variance of the solution depends on the boundary conditions imposed. Estimates of the variance of the solution is presented both analytically and numerically. The technique is used on both a simple model problem as well as the one-dimensional Euler and Navier-Stokes equations.

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MS3

A Dynamically Bi-Orthogonal Method for Time-Dependent Stochastic Partial Differential Equation

We propose a dynamically bi-orthogonal method (DyBO) to study time dependent stochastic partial differential equations (SPDEs). The objective of our method is to exploit some intrinsic sparse structure in the stochastic solution by constructing the sparsest representation of the stochastic solution via a bi-orthogonal basis. In this talk, we derive an equivalent system that governs the evolution of the spatial and stochastic basis in the KL expansion. Several numerical experiments will be provided to demonstrate the effectiveness of the DyBO method.

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MS4

Recursive Estimation Procedure of Sobol Indices based on Replicated Designs

In the context of global sensitivity analysis, the estimation procedure based on replicated designs, denoted by replication procedure, allows to estimate Sobol' indices at an efficient cost. However this method still requires a large number of model evaluations. Here, we consider the ability of increasing the number of evaluation points, thus the accuracy of estimates, by rendering the replication procedure recursive. The key feature of this approach is the construction of structured space-filling designs. For the estimation of first-order indices, we exploit a nested Latin Hypercube already introduced in the literature. For the estimation of closed second-order indices, we propose an iterative construction of an orthogonal array of strength two. Various space-filling criteria are used to evaluate our designs.

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MS4

Generation of Tailor-Made Regular Factorial Designs

Many factorial designs used in practice belong to the class of regular designs, whose construction is based on properties of finite abelian groups. Regular factorial designs can be adapted to a large diversity of situations with respect to the input factors. I will talk about the automatic generation of regular designs based on practical user's specifications, and discuss how it can be applied to the design of computer experiments.

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MS4

Some New Space-Filling Designs for Computer Experiments

Orthogonal arrays provide an attractive class of space-filling designs for computer experiments. In this talk, I will present several new classes of space-filling designs, which enjoy better space-filling properties than ordinary orthogonal arrays. Of the main focus are strong orthogonal arrays and mappable nearly orthogonal arrays.

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MS4

Experimental Design Principles in Quadrature for Uncertainty Quantification

The sparse quadrature grids at which functions are evaluated for quadrature In UQ can be considered as experimental design points. An example is in estimating the coefficients of a polynomial chaos expansion. This prompts the use, and combination, of several areas of experimental design in UQ: (i) algebraic statistics (using Groebner bases) applied to the problem of which multivariate moments can be estimated (ii) optimal and space-filling designs for computer experiments.

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MS5

Map Estimators and Their Consistency in Bayesian Inverse Problems for Functions

We consider the inverse problem of estimating an unknown function from noisy measurements of a known, possibly nonlinear map of the unknown function. Under certain conditions, the Bayesian approach to this problem results in a well-defined posterior measure. Under these conditions, we show that the maximum a posteriori (MAP) estimator is characterised as the minimiser of an Onsager-Machlup functional on an appropriate function space depending on the prior. We then establish a form of Bayesian posterior consistency for the MAP estimator.

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MS5

The Bayesian Formulation of EIT: Analysis and Algorithms

We provide a rigorous Bayesian formulation of the EIT problem in an infinite dimensional setting, leading to well-posedness in the Hellinger metric with respect to the data. We focus particularly on the reconstruction of binary fields where the interface between different media is the primary unknown. We consider three different prior models - log-Gaussian, star-shaped and level set. Numerical simulations based on the implementation of MCMC are performed, illustrating the advantages and disadvantages of each type of prior in the reconstruction, in the case where the true conductivity is a binary field, and exhibiting the properties of the resulting posterior distribution.

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MS5

Maximum a Posteriori Estimates in Bayesian Inverse Problems

We discuss the maximum a posteriori (MAP) estimate and its definition for infinite-dimensional non-Gaussian Bayesian inverse problems. Moreover, we consider how Bregman distance can be used to characterize the MAP estimate.

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MS5

Approximations of Bayesian Inverse Problems Using Gaussian Process Emulators

A major challenge in the application of Markov chain Monte Carlo methods to large scale inverse problems, is the high computational cost associated with solving the forward model for a given set of input parameters. To overcome this difficulty, we consider using a surrogate model that approximates the solution of the forward model at a much lower computational cost. We focus in particular on Gaussian process emulators, and analyse the error in the posterior distribution resulting from this approximation.

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MS6

Stability of and Preconditioners for the Pressure and Velocity Reconstruction Based on Coarse and Noisy Velocity Measurement Such As 4D Phase-Contrast Magnetic Resonance Imaging

Modern imaging such as Phase-Contrast Magnetic Resonance Imaging provide 4D images of blood flow in for example cerebral aneurysms. The problem, however, is that the resolution in both space and time is coarse and subject to noise. This makes important quantities like pressure or wall-shear stress difficult to compute by local considerations. Therefore, we will in this talk consider the subject of reconstructing high-resolution velocities and pressure by solving optimal control problems subject to PDEs for the fluid flow.

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MS6

Statistical Inverse Problems with Application to Neurosciences

Spatial regression with differential regularization is a novel class of models for the accurate estimation of surfaces and spatial fields, that merges advanced statistical methodology and scientific computing techniques. The proposed models efficiently handle data distributed over irregularly shaped domains and manifold domains and allow for a very flexible modeling of the space variation. Full uncertainty quantification is available via classical inferential tools. The method is illustrated via application to neuroimaging data.

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MS6

Understanding the Effects of Internal Carotid Artery Flow Uncertainty on Intracranial Aneurysm Haemodynamics: an "In Silico" Study on a Virtual Population

Inter-subject variations of systemic flow waveforms could influence vascular wall response in intracranial aneurysms and consequently the progression of the disease. In this work, flow waveform variability is quantified using a virtual waveform population, generated by Gaussian process model. Computational fluid dynamics simulations map this virtual population onto the aneurysmal wall shear stress space. Surrogate models and sparse grid sampling are used to explore the flow uncertainty related to distal outlet branch resistances and compliances.

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MS6

Impact of Material Parameter Uncertainty on Stress in Patient Specific Models of the Heart

In this talk we study the impact of material parameter uncertainty on stress computations in patient specific models of the heart. Stress is a driver of pathological remodeling, and stress estimates may therefore have substantial clinical value. The computations rely on parameters that must be estimated from medical image data, and which typically contain a large degree of uncertainty. We present methods for parameter estimation, and study the impact of parameter variation on myocardial stress.

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MS7

Statistical Stopping Rules for Iterative Inverse Solvers

Iterative linear system solvers have been shown to be regularization methods when equipped with a suitable stopping rule. In this talk we propose new statistical stopping criteria that provides a measure of the uncertainty in the solution.

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MS7

Stochastic Boundary Maps in Eit

Electrical impedance tomography (EIT) is considered in a setting where the computational domain with an unknown conductivity distribution comprises only a portion of the whole conducting body, and a boundary condition along the artificial boundary needs to be set in order to minimally disturb the estimate in the domain of interest. The boundary map at the artificial boundary is an additional unknown that needs to be estimated along with the conductivity of interest.

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MS7

Inverse Boundary Value Problem of Thermal Tomography

We consider the inverse parabolic boundary value problem of thermal imaging. The corresponding forward problem is first solved by using the stochastic finite element method. The heat capacity and the thermal conductivity are then reconstructed simultaneously by minimizing a chosen Tikhonov-type functional. Only polynomial evaluation and differentiation are required during the inversion, which makes the method fast. Numerical examples are presented in two spatial dimensions with uncertain boundary curve.

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MS7

Statistical Methods for Pricing and Risk Manage-

ment of CoCo-bonds

Substantial amounts of contingent convertible (CoCo) bonds have recently been issued by banks to guarantee the minimum capital requirements of the Basel III regulations. Mark-to-model pricing of such instruments poses challenges from modeling and calibration perspectives. We present a smile-conform generalization of the Black and Scholes equity derivatives modeling approach. We formulate the corresponding calibration problem as a statistical inverse problem and discuss numerical aspects as well as the usefulness of such an approach with regard to risk management.

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MS8

Review of Uq in Turbulence Modelling to Date

We give an overview of stochastic techniques in turbulence modeling, including outlining the major motivations, issues, techniques and applications. We aim to provide a context within which the following talks can be understood.

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MS8

Quantifying Model-Form Uncertainties Using Field Inversion and Machine Learning

The dominant source of error in turbulence models is because of structural inadequacies in the model. In this work, full-field inversion is used to obtain corrective, spatially distributed functional forms of model discrepancies in a wide class of problems. Once the inference has been performed over a number of problems that are representative of the deficient physics in the closure model, machine learning techniques are used to reconstruct the model corrections in terms of variables that are accessible in the closure model. The problem is cast in a Bayesian setting and is shown to effectively represent model-form errors in a predictive setting.

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MS8

A Practical Method for Estimating Uncertainty Due to Rans Modeling

Bayesian Model Scenario Averaging (BMSA) combines multiple RANS turbulence models and posterior closure coefficient distributions to obtain a stochastic estimate of a Quantity of Interest for an unmeasured prediction scenario. However, the full BMSA approach requires many forward samples, which can prohibit its application to complex flow topologies. Therefore, we present a simplified version of BMSA based on Maximum a Posteriori estimates, and apply it to a transonic flow over a 3D wing.

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MS8

A Stochastic Model Inadequacy Representation for a Reynolds-Averaged Burgers' Equation K-Epsilon Model

We perform Reynolds' averaging to a random Burgers' Equation and close the equation with an $k-\varepsilon$ eddy viscosity model. A stochastic model inadequacy formulation is developed in which a stochastic PDE governs the error in the computed Reynolds stress. This formulation is based on an exact equation for the Reynolds stress but includes random forcing to represent uncertainty due to the turbulence model. The inadequacy model is calibrated with Bayesian methods and compared to data.

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MS9

Data Assimilation, Parameter Estimation and Rom for Cardiovascular Flows

We present a complete framework combining data assimilation from real medical (patient-specific) data, numerical simulation carried out by high performance infrastructure and its combination with reduced order modelling methodologies in order to guarantee competitive computational costs and real-time computing. Parameters estimation is another important goal, as well as parametric sensitivity analysis in the worst medical scenario. Several examples are discussed to introduce recent advances in reduced order methodology and its properties.

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MS9

Space-TimeAdaptive Approach to Variational Data Assimilation Using Wavelets

This talk focusses on one of the main challenges of 4-dimensional variational data assimilation, namely the requirement to have a forward solution available when solving the adjoint problem. The issue is addressed by considering the time in the same fashion as the space variables, reformulating the mathematical model in the entire space-time domain, and solving the problem on a near optimal computational mesh that automatically adapts to spatio-temporal structures of the solution. The compressed form of the solution eliminates the need to save or recompute data for every time slice as it is typically done in traditional time marching approaches to 4-dimensional variational data assimilation. The reduction of the required computational degrees of freedom is achieved using the compression properties of multi-dimensional second generation wavelets. The simultaneous space-time discretization of both the forward and the adjoint models makes it possible to solve both models either concurrently or sequentially. In addition, the grid adaptation reduces the amount of saved data to the strict minimum for a given a priori controlled accuracy of the solution. The proposed approach is demonstrated for the advection diffusion problem in two space-time dimensions.

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MS9

Non Intrusive Polynomial Chaos Using Model Reduction

This work proposes a new efficient method for estimating uncertainty propagation. We investigate time-dependent viscous Burgers equation. The viscosity parameter is assumed to be an uncertain quantity with normal distribution of known mean and variance. A stochastic Galerkin projection is performed on a truncated polynomial chaos (PC) expansion of Hermite polynomials. Smolyak sparse interpolation method and first and second order adjoint techniques are applied to accelerate the spectral collocation PC. In addition, a dictionary of local parametric reduced order models with known error estimates are used to increase the method efficiency too since multiple solutions of the original model (deterministic) model are required. Finally we compare results and CPU load against Monte Carlo outcomes.

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MS9

Non-smooth Optimization Techniques for Solving a Radiation Data Assimilation Problem

Detection of radiation release events in an urban environment requires efficient strategies to accurately identify and track the threat to the urban population in the proximity of the event. This work proposes to estimate the location and intensity of a simulated radiation source located in a Washington DC neighborhood. Due to the domain geometry and the source to sensor radiation model employed in this study the quadratic cost function associated with this problem presents multiple discontinuities and local minima. Non-smooth optimization techniques including Implicit Filtering, Nelder-Mead, Genetic Algorithm and Simulated Annealing have the potential to deal with such difficulties and their performances are compared for computational efficiency.

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MS10

Fracture Length and Aperture Correlations: Implications for Transport Simulations in Discrete Fracture Networks

Abstract not available.

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MS10

Decision-Oriented Optimal Experimental Design

Abstract not available.

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MS10

Using Level-Set Methods to Generate Random Conductivity Fields Conditioned on Data and De-

sired Statistical and Geometric Characteristics

Abstract not available.

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MS10

Inversion by Conditioning

Abstract not available.

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MS11

Ensemble Grouping Strategies for Embedded Stochastic Collocation Methods Applied to Anisotropic Diffusion Problems

In this presentation we propose a method for the solution of a stochastic elliptic PDE with an uncertain diffusion parameter featuring high anisotropy. In the context of stochastic collocation finite element methods we use a local hierarchical polynomial approximation with respect to the uncertain parameters in the sample space. The deterministic PDEs are solved by propagating ensembles of samples in an embedded fashion; we explore different sample-grouping techniques and compare their performance.

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MS11

A Multilevel Stochastic Collocation Method for Pdes with Random Inputs

Abstract not available.

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MS11

Embedded Ensemble Propagation for Improving Performance, Portability and Scalability of Uncertainty Quantification on Emerging Computational Architectures

Typical approaches for forward uncertainty propagation involve sampling of computational simulations over the range of uncertain input data. Often simulation processes from sample to sample are similar. We explore a rearrangement of sampling methods to simultaneously propagate ensembles of samples in an embedded fashion. We demonstrate this enables reuse between samples, reduces computation and communication costs, and improves opportunities for fine-grained parallelization, resulting in improved performance on a variety of contemporary computer architectures.

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MS11

A Reduced-Basis Multilevel Method for High-Dimensional Stochastic Systems

We combine multi-level Monte Carlo (MLMC) sampling strategy with complexity reduction techniques, POD and reduced basis. Reduced models dramatically lower the computational cost of PDE realizations, but often suffer from limited accuracy. MLMC offers a robust framework for exploiting multi-fidelity models, however, thus far, the application of MLMC has been restricted to various discretization schemes. Our approach combines model reduction techniques with MLMC, thus arbitrary accuracy can be achieved at a very low computational cost.

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MS12

Infinite-Dimensional Compressed Sensing and Function Interpolation

We introduce a framework for function interpolation using compressed sensing with weighted l1 minimization. Unlike previous results, our recovery guarantees are sharp for large classes of functions regardless of the weights used. They also allow one to determine an optimal weighting strategy in the case of multivariate polynomial approximations in lower sets. Finally, we use these guarantees to establish the benefits of a well-known weighting strategy where the weights are chosen based on prior support information.

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MS12

Gradient-enhanced ℓ_1-minimization for Stochastic Collocation Approximations

This work is concerned with stochastic collocation methods via gradient-enhanced ℓ_1-minimization, where the derivative information is used to identify the Polynomial Chaos expansion coefficients. With an appropriate preconditioned matrix and normalization, we show the inclusion of derivative information will lead to a successful solution recovery, both for bounded and unbounded domains. Numerical examples are provided to compare the computational perfomance between standard ℓ_1-minimization and the gradient-enhanced ℓ_1 minimization. Numercl results suggest that including derivative information can accelerate the recovery of the PCE coefficients.

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MS12

Stability and Accuracy of the Discrete Least-squares Approximation on Multivariate Polynomial Spaces

We review the main results achieved in the analysis of the stability and accuracy of the discrete least-squares approximation on multivariate polynomial spaces, with noiseless evaluations at random points, noiseless evaluations at low-discrepancy point sets, and noisy evaluations at random points.

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MS12

Stochastic Collocation with Multi-Fidelity Models

We shall discuss a numerical approach for the stochastic collocation method with multi-fidelity simulation models. The method combines the computational efficiency of low-fidelity models with the high accuracy of high-fidelity models. When incorporating the idea of control variates, we exploit the statistical correlation between the low-fidelity and high-fidelity model to accelerate the convergence of the standard multi-fidelity approximation. We shall present several numerical examples to demonstrate the efficiency and applicability of the multi-fidelity algorithm.

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MS13

Sparse Grid, Reduced Basis Bayesian Inversion

In this talk, we present a computational reduction framework for efficient and accurate solution of Bayesian inverse problems that commonly face the curse of dimensionality and large-scale computation. For the approximation of high or infinite dimensional integration, we take advantage of the sparsity that can be automatically detected by a dimension-adaptive sparse grid construction. In harnessing the large-scale computation, we exploit the reducibility of high-fidelity approximation and propose a goal-oriented reduced basis method. This framework features considerable reduction of the computational cost for solving Bayesian inverse problems of a large range of parametric operator equations.

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MS13

Goal-Oriented Nonlinear Model Reduction for Fast Bayesian Inference

This work describes a novel approach for inverting the true characterization of large-scale and non-Gaussian random field from noisy measurements, with the help of verified and validated simulations of the underlying physical processes. We will investigate innovative goal-oriented nonlinear dimension reduction methods based on kernel principal component analysis as well as adjoint methods for fast Bayesian inference. We will demonstrate the approach by applying it to recovering the probabilistic distribution of a channelize permeability field.

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MS13

Nonlinear Reduced-Order Models for Unsteady

Compressible Flows

There are many theoretical and practical challenges in developing accurate and efficient reduced-order models for nonlinear compressible flow. This talk will describe ideas developed to meet these challenges and their implementation in a Sandia in-house CFD solver. This work focuses on projection-based Galerkin and Petrov-Galerkin model reduction methods with hyper-reduction with the goal of employing these ROMs for uncertainty quantification of unsteady compressible flows.

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MS13
Control for Systems with Uncertain Parameters

We consider PDE systems that depend on a parameter (i.e. viscosity) that is critical for the dynamics and stability of the plant. By using a mixture of classical optimal control techniques combined with data-driven reduced order model updates, we obtain accurate online models for control. We present a strategy, where the control action can respond to failure scenarios through significant updates to the feedback gains.

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MS14
Low-Rank Tensor Approximations in Reduced Basis Methods and Uncertainty Quantification

We propose a novel combination of the reduced basis method with low-rank tensor techniques for the efficient solution of parameter-dependent linear systems in the case of several parameters, as they arise, for example, in uncertainty quantification. This combination consists of three ingredients. First, the underlying parameter-dependent operator is approximated by an explicit affine representation in a low-rank tensor format. Second, a standard greedy strategy is used to construct a problem-dependent reduced basis. Third, the associated reduced parametric system is solved for all parameter values on a tensor grid simultaneously via a low-rank approach. This allows us to explicitly represent and store an approximate solution for all parameter values at a time. Once this approximation is available, the computation of output functionals and the evaluation of statistics of the solution becomes a cheap online task, without requiring the solution of a linear system.

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MS14
Block-Diagonal Preconditioning for Optimal Control Problems Constrained by PDEs with Uncertain Inputs

We present an efficient approach for simulating optimization problems governed by partial differential equations involving random coefficients. This class of problems leads to prohibitively high dimensional saddle point systems with Kronecker product structure, especially when discretized with the stochastic Galerkin finite element method. Here, we derive and analyze robust Schur complement-based block diagonal preconditioners for solving the resulting stochastic Galerkin systems with low-rank iterative solvers. Finally, we illustrate the effectiveness of our solvers with numerical experiments.

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MS14
Fast Solvers for Parameter-Dependent Pdes

The first talk of this two-part mini-symposium is intended to be an introduction. I will give an overview of the computational challenges associated with solving the linear systems of equations associated with various numerical methods for discretizing parameter-dependent PDEs and/or PDEs with random inputs. The talk is intended to set up the other seven in the mini-symposium by covering concepts like low-rank and reduced basis iterative solvers, preconditioning for matrices with Kronecker product structure, and optimal stopping criteria.

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MS14
An Efficient Reduced Basis Solver for Stochastic Galerkin Matrix Equations

Stochastic Galerkin FE approximation of PDEs with random inputs leads to linear systems with characteristic Kronecker product structure coefficient matrix. By reformulating the systems as multi-term linear matrix equations, we develop an efficient solution algorithm which generalizes ideas from rational Krylov subspace projection methods. Its convergence rate is independent of the spatial approximation, while its memory requirements are far lower than those of the preconditioned conjugate gradient applied to the Kronecker formulation of the systems.

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MS15

Adaptive Methods for Pde Constrained Optimization with Uncertain Data

I present an approach to solve risk averse PDE constrained optimization problems with uncertain data that uses different PDE model fidelities and adaptive sampling to substantially reduce the overall number of costly, high fidelity PDE. The approximation qualities of the optimization subproblems due to sampling and lower fidelity PDE models is adjusted to the progress of the overall optimization algorithm.

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MS15

Stochastic Collocation for Optimal Control with Stochastic Pde Constraints

We discuss the use of stochastic collocation for the solution of optimal control problems which are constrained by stochastic partial differential equations (SPDE). Thereby the constraining SPDE depends on data which is not deterministic but random. Assuming a deterministic control, randomness within the states of the input data will propagate to the states of the system. For the solution of SPDEs there has recently been an increasing effort in the development of efficient numerical schemes based upon the mathematical concept of generalized Polynomial Chaos. Modal-based stochastic Galerkin and nodal-based stochastic collocation versions of this methodology exist, both of which rely on a certain level of smoothness of the solution in the random space to yield accelerated convergence rates. In the talk we show how to apply the stochastic collocation method in a gradient descent as well as a sequential quadratic program (SQP) for the minimization of objective functions constrained by an SPDE. The stochastic function involves several higher-order moments of the random states of the system as well as classical regularization of the control. In particular we discuss several objective functions of tracking-type. To demonstrate the performance of the method we show numerical test examples and we give an outlook to a real-world problem from medical treatment planning.

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MS15

Mean-variance Risk-averse Optimal Control of Systems Governed by PDEs with Random Parameter Fields using Quadratic Approximations

We present a method for risk-averse optimal control of systems governed by PDEs with uncertain parameter fields. To make the problem computationally tractable, we invoke a quadratic Taylor series approximation of the control objective with respect to the uncertain parameter field. This enables deriving explicit expressions for the mean and variance of the control objective in terms of its gradients and Hessians with respect to the uncertain parameter. The proposed approach is illustrated using an elliptic PDE control problem with uncertain coefficient, and we present a comprehensive numerical study.

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MS15

Low-Rank Solvers for An Unsteady Stokes-Brinkman Optimal Control Problem with Random Data

We consider the simulation of an optimal control problem constrained by the unsteady Stokes-Brinkman equation involving random data. We consider a generalized polynomial chaos approximation of these random functions in the stochastic Galerkin finite element method. The discrete problem yields a prohibitively high dimensional saddle point system with Kronecker product structure. We discuss how such systems can be solved using tensor-based methods. The performance of our approach is illustrated with extensive numerical experiments.

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MS16

Generalized Rybicki Press Algorithm in Higher Dimensions

Covariance matrices whose elements are sums of exponentials are frequently encountered in computational statistics in the context of Continuous time AutoRegressive-Moving-Average. The talk discusses a more general, numerically stable, linear complexity Rybicki Press algorithm for such matrices. The algorithm which enables inverting and computing determinants of covariance matrices scales as $O(N^{(3d-2)/d})$ in exact arithmetic. In finite arithmetic, the algorithm scales as $O(N)$ and offers more compressibility than the typical fast direct solvers. Detailed benchmarks illustrate the scaling of the algorithm in various dimensions.

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MS16

Hierarchically Compositional Kernels for Scalable Nonparametric Learning

We propose a novel class of kernels to alleviate the high computational cost of large-scale nonparametric learning with kernel methods. The proposed kernel marries the Nyström method with a locally lossless approximation in a hierarchical fashion and maintains positive-definiteness. We demonstrate comprehensive experiments to show its effectiveness. In particular, on a laptop and a dataset with approximately half a million training examples, the proposed kernel achieves a performance close to that of the nonapproximate kernel by using less than two minutes of training.

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MS16

Fitting Gaussian Processes in Ensemble Kalman Filters

Ensemble Kalman filters have become popular for data assimilation in high-dimensional non-linear systems. The methods rely on propagating Monte Carlo samples, and constructing an empirical Gaussian approximation when integrating (dynamic) data. Because of the empirical approximations, samples get coupled over integration steps, and the approach often underestimates the prediction variance. Several approaches have been suggested to mitigate this challenge; localization, inflation, dimension reduction, etc. We here suggest to fit an approximation by estimating the covariance parameters of a Gaussian process. We compare various methods using spatial blocking schemes, and non-stationary models. We show applications from Earth sciences.

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MS16

Fast Spatial Gaussian Process Maximum Likelihood Estimation Via Skeletonization Factorizations

We present a procedure for sets of n unstructured 2D observations for evaluation of the kernelized Gaussian process log-likelihood and gradient in $\tilde{\mathcal{O}}(n^{3/2})$ time and $\mathcal{O}(n \log n)$ storage. Our method uses the skeletonization procedure described by Martinsson & Rokhlin (2005) in the form of the *recursive skeletonization factorization* of Ho & Ying (2015). We combine this with the matrix peeling algorithm of Lin et al. (2011) to compute maximum-likelihood estimates using black-box optimization packages.

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MS17

Dealing with Uncertainties in Global Decadal Ocean State Estimation

Over the last 1.5 decades the consortium "Estimating the Circulation and Climate of the Ocean" (ECCO) has developed a framework for fitting a state of the art global ocean (and sea ice) general circulation model (GCM) to much of the available diverse streams of satellite and in situ observations via a deterministic least-squares approach. A key ingredient is the availability of an adjoint model of the time-evolving GCM to invert for uncertain initial and surface boundary conditions, as well as internal model parameters. With increasing maturity of the framework and the decadal global state estimates produced, increased attention is warranted to assess the fidelity of prior errors assigned to the observations and the inversion (control) variables, as well as a rigorous assessments of posterior uncertainties. The latter is a key open question, both for the provision of realistic uncertainties in climate reconstructions, as well as implications for forecasting. Ongoing work to tackle these problems in the context of ECCO will be described.

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MS17

UQ for the Global Atmosphere Using Concurrent Samples

A universal problem facing all scientific computing applications is how to achieve efficient calculations on emerging architectures. Uncertainty quantification imposes the need for ensembles of simulations. It also provides a potential source of additional computational work on each compute node by computing these ensemble samples concurrently, i.e. as an inner loop rather than an outer loop. We present results for this approach for a global atmosphere model being developed at Sandia National Laboratories.

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MS17

The Importance of Being Uncertain: The Influence of Initial Conditions in Ocean Models

This paper describes how we might quantify the initial contributions to overall model uncertainty. We test our assumptions about the uncertainty of the initial conditions by designing a robust sampling scheme of the inputs and use selected inputs to run a set of global Community Earth System Model (CESM) simulations. Using Bayesian statistics, the selective inputs and associated outputs are used to interpolate outcomes to produce a broad distribution of uncertainty in a given metric.

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MS18

Asymptotic-Preserving Stochastic Galerkin Schemes for the Boltzmann Equation with Uncertainty

We develop a stochastic Galerkin method for the nonlinear Boltzmann equation with uncertainty. The method is based on the generalized polynomial chaos (gPC) and can handle random inputs from collision kernel, initial data or boundary data. We show that a simple singular value decomposition of gPC related coefficients combined with the Fourier-spectral method (in velocity space) allows one to compute the collision operator efficiently. When the Knudsen number is small, we propose a new technique to overcome the stiffness. The resulting scheme is uniformly stable in both kinetic and fluid regimes, which offers a possibility of solving the compressible Euler equation with random inputs.

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MS18

An Adaptive Hybrid Stochastic Galerkin Method for Uncertainty Quantification for Hyperbolic Problems with Several Random Variables

The continuous sedimentation process in a clarifier-thickener can be described by a scalar non-linear conservation law. The applications of this model on the realistic setting requires the dealing with several uncertain parameters. Therefore the numerical simulation of this problem requires an efficient method of the uncertainty quantification. The presented hybrid stochastic Galerkin (HSG) method extends the classical polynomial chaos approach by multiresolution discretization in the stochastic space. The HSG approach leads to a partially decoupled deterministic hyperbolic system, which allows an efficient parallel numerical simulation. The numerical approximation of the solution of the resulting high-dimensional hyperbolic system is provided by the introduced finite-volume scheme. The multi-wavelet based stochastic adaptivity provides the further reduction of the problem complexity. Several presented numerical experiments show the application of the HSG method on the clarifier-thickener problem with several random parameters and demonstrate advantages of the method.

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MS18

Control Problems in Socio-Economic Models with Random Inputs

Abstract not available.

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MS18

Stochastic Regularity of Observables for High Frequency Waves

We consider high frequency waves satisfying the scalar wave equation with highly oscillatory initial data. The speed of propagation of the medium as well as the phase and amplitude of the initial data is assumed to be uncertain, described by a finite number of independent random variables with known probability distributions. We introduce quantities of interest (QoIs) as local averages of the squared modulus of the wave solution, or its derivatives. In the talk we will discuss the regularity of these QoIs in terms of the input random parameters, and the wave length. The regularity is important for uncertainty quantification methods based on interpolation in the stochastic space. In particular, the stochastic regularity should, in an appropriate sense, be independent of the wave length. We show that the QoIs can indeed have this property, despite the highly oscillatory character of the waves.

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MS19

Inference for Multi-Model Ensembles: An Application in Glaciology

Computational models are frequently used to explore physical systems. Often, there are several computer models available and also a limited number of observations from the physical system. Here, new methodology is proposed for combining multiple computational models and field observations to make predictions for the system with uncertainty. We do not choose a best model, but instead use a spatially varying convex combination of models. The methodology is motivated by an application in glaciology.

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MS19

Optimal Design for Correlated Processes with Input-Dependent Noise

We present a design criterion for parameter estimation in Gaussian process regression models with input-dependent noise. The motivation stems from the area of computer experiments, where computationally demanding simulators are approximated using Gaussian process emulators. Designs are proposed with the aim of minimising the variance of heteroscedastic Gaussian process parameter estimation. A Gaussian process model is presented which allows for an experimental design technique based on an extension of Fisher information to heteroscedastic models.

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MS19

Combination of Sequential Design and Variable Screening. Application to Uncertainties in the Source of Tsunami Simulations

There is a computational advantage in building a design of computer experiments solely on a subset of active variables. However, this prior selection inflates the limited computational budget. We propose to interweave the recent sequential design strategy MICE (Mutual Information for Computer Experiments) with a screening algorithm to improve the overall efficiency of building an emulator. This approach allows us to assess future tsunami risk for complex earthquake sources over Cascadia using the simulator VOLNA.

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MS19

Design for Calibration and History Matching for Complex Simulators

Design for building emulators of computer experiments usually focusses on how to build accurate global approximations. However, if our aim is calibration, then this can be wasteful. In this talk I will discuss design strategies that can be used for history matching and calibration, both in a deterministic and stochastic setting. Entropy based designs that minimize the uncertainty in the classification surface are particularly useful, and we will show how these can be efficiently computed.

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MS20

Optimal Experimental Design for Large-Scale PDE-Constrained Nonlinear Bayesian Inverse Problems

We address the problem of optimal experimental design (OED) for infinite-dimensional nonlinear Bayesian inverse problems. We seek an A-optimal design, i.e., we aim to minimize the average variance of a Gaussian approximation to the inversion parameters at the MAP point. The OED problem includes as constraints the optimality condition PDEs defining the MAP point as well as the PDEs describing the action of the posterior covariance. We provide numerical results for the inference of the permeability field in a porous medium flow problem.

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MS20

Advances in Dimension-independent Markov Chain Monte Carlo Methods

This talk concerns Markov chain Monte Carlo (MCMC) algorithms whose performance is independent of the dimension of the underlying state-space, in an appropriate sense. The first part of the talk concerns function-space MCMC algorithms for sampling the posterior distribution arising from Bayesian inverse problems. A general class of operator-weighted proposal distributions are introduced, which are dimension(and covariance)-independent, and may include local gradient information. These proposals utilize Hessian information to identify a subspace in which the posterior measure concentrates, and adaptively scale the proposal distribution according to the posterior covariance in this space. The high level of efficiency of these algorithms is demonstrated numerically on examples. Time permitting, the second part of the talk will describe recent advances, exploiting many-core architectures combined with GPU accelerators, which illustrate the potential for gradient-free adaptive MCMC algorithms to efficiently explore targets over high-dimensional state spaces, which may not arise from the discretization of a function space.

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MS20

Multilevel Sampling Techniques for Bayesian Inference

Multilevel sampling methods, for example within a Metropolis-Hastings algorithm or as ratio estimators for Bayes' formula, are among the most efficient methods for large-scale PDE-constrained Bayesian inference. Through a clever use of model hierarchies – naturally available in the numerical approximation of PDEs – they offer the accuracy of "gold-standard" classical MCMC estimators at a fraction of the cost, avoiding dimension truncation, Gaussian approximations or linearisations. We present theory and numerical experiments.

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MS20

Metropolis-Hastings Algorithms in Function Space for Bayesian Inference of Groundwater Flow

We consider a class of Metropolis-Hastings algorithms suited for general Hilbert spaces and their application to Bayesian inference in PDE models. In particular, we generalize the existing pCN-proposal in order to allow for adaption to the posterior covariance. This improves the statistical efficiency and numerical experiments indicate that the new method performs independent of dimension and noise variance. We further provide a convergence result for the proposed MH algorithms in terms of spectral gaps.

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MS21

A Reduced-Order Strategy for Efficient State/parameter Identification in Cardiac Electrophysiology

A reduced basis (RB) ensemble Kalman filter is proposed for solving efficiently inverse UQ problems in cardiac electrophysiology. Our goal is to identify the location and shape of ischemic regions, affecting the coefficients of a nonlinear unsteady PDE which models the evolution of the cardiac potential. Combining a RB method for state reduction and a reduction error model for the sake of reliability we can speedup both sampling and updating of parameters probability distributions.

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MS21

A Moment-Matching Method to Study the Variability of Phenomena Described by Complex Models

A stochastic inverse problem is proposed aiming at studying the observed variability of phenomena. Given an experimental setup and a parametric model, the probability density of the parameters is estimated by imposing that the statistics of the model outputs match the measured ones. An entropy regularisation formulation of the problem is adopted, and numerically solved by a stochastic collocation approach. The method is tested on various test cases, including experiments in cardiac electrophysiology.

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MS21

Data Assimilation and Uncertainty Quantification for Surgery Planning of Single-Ventricle Pathophysiology

Blood flow simulations for surgery planning are typically based on preoperative patient data. Thus the first step consists in performing data assimilation on an appropriate reduced model which represents the circulation outside of the 3D domain of interest, and which is coupled to it. Through cases of single-ventricle pathophysiology, we will present two different strategies to estimate such parameters and take into account the uncertainties in the measurements.

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MS21

Bayesian Multi-Fidelity Monte Carlo for Uq with Large-Scale Models

We propose a novel Bayesian multi-fidelity uncertainty quantification scheme for complex systems with high stochastic dimension, which achieves unrivalled efficiency through rigorous incorporation of information from low-fidelity models. These need not to be accurate in a deterministic sense; merely a similar stochastic structure needs to be retained by the low-fidelity model. We demonstrate the capabilities of our approach through its application to complex, large-scale biomechanical models of abdominal aortic aneurysms and the human respiratory system.

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MS22

Novel Uncertainty Measures for Inverse Problems

Uncertainty quantification is measured by variances or mean-squared errors, which makes perfect sense in a Hilbert space framework respectively Bayesian posteriors close to Gaussians. For different underlying geometries far from Hilbert spaces and posteriors far from Gaussian, the meaning of such measures is questionable and often not even defined in an infinite-dimensional limit. In this talk we therefore consider different measures for uncertainty quantification based on Banach spaces, there duals, and Bregman distances related to the norm. We discuss their properties and their potential use in uncertainty quantification, in particular related to variational methods in inverse problems and imaging.

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MS22

Stochastic Inverse Problems with Impulsive Noise

Impulsive noise models such as salt & pepper noise are frequently used in mathematical image restoration, but are usually restricted to the discrete setting. We introduce an infinite-dimensional stochastic impulsive noise model based on marked Poisson point processes, discuss its properties and show regularization properties of inverse problems subject to such noise. We also treat the conforming discretization of such noise models and compare this to the classical discrete impulsive noise.

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MS22

Stochastic Modulus of a Quadrilateral As a Benchmark Problem for Uncertain Domains

We consider the stochastic version of the classical capacity problem for uncertain domains. For this problem, there exists a natural error estimate for any realization of any random boundary. This so-called reciprocal error estimate can be used in the error analysis of statistical quantities related to the numerical solution of the model problem by using a sparse grid stochastic collocation method, where the error estimate is applied to each individual solution within the non-intrusive process.

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MS22

Convergence Rates for Bayesian Inversion

Let us consider an indirect noisy measurement M of a physical quantity U;

$$M = AU + \delta\mathcal{E},$$

where the measurement M, noise $\mathcal{E}$ and the unknown U are treated as random variables and δ models the noise amplitude. We are interested to know what happens to the approximate solution of above when $\delta \to 0$. The analysis of small noise limit, also known as the theory of posterior consistency, has attracted a lot of interest in the last decade, however, much remains to be done. Developing a comprehensive theory is important since posterior consistency justifies the use of the Bayesian approach the same way as convergence results do the use of regularisation techniques. This is joint work with Matti Lassas and Samuli Siltanen

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MS23

Quantifying Turbulence Model Form Uncertainty in Rans Simulations of Complex Flow and Scalar Transport

Reynolds-averaged Navier-Stokes (RANS) simulations offer a practical approach for engineering analysis of turbulent flows, but the uncertainty related to the turbulence model should be quantified when using the results for design decisions. Previously we demonstrated promising capabilities of an approach that quantifies the uncertainty in turbulence and turbulent scalar flux models by perturbing the modeled quantities in the governing equations. This presentation will discuss recent findings from applying the methodology to different complex flow configurations.

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MS23

Machine Learning for Uncertainty Quantification in Turbulent Flow Simulations

Because Reynolds Averaged Navier Stokes (RANS) simulations rely on turbulence model closures, the simulation predictions are prone to increased uncertainty in flows where the underlying model assumptions are invalid. Machine learning methods, in combination with the big data sets generated by high fidelity simulations, can be leveraged to detect when these underlying assumptions are violated. This presentation will discuss feature selection methods, machine learning algorithm performance, extrapolation metrics, and rule extraction techniques in the context of RANS model form uncertainty quantification.

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MS23

Uncertainty Quantification and Sensitivity Analysis in Large-Eddy Simulations

The assessment of the quality and reliability of large-eddy simulation (LES) results is difficult, because different sources of uncertainty/errors, such as modeling or numerical discretization, may have comparable effects. We use UQ to address the sensitivity of LES results to grid resolution and SGS modeling, by assuming the uncertain parameters as input random variables. Continuous response surfaces in the parameter space are built from a small number of LES simulations by using a surrogate model, as e.g the gPC approach.

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MS23

Combining Approximate and Exact Bayesian Algorithms to Quantify Model-Form Uncertainties in RANS Simulations

Properly quantifying model-form uncertainties in RANS simulations is important yet challenging. In this work, we propose a physics-informed Bayesian framework to address this problem. Uncertainties are introduced directly to the Reynolds stresses, and are parameterized accounting for empirical prior and physical constraints. A hybrid inversion scheme is adopted based on Ensemble Kalman method and MCMC method, where a surrogate model is employed to reduce the computational cost. Two test cases are performed to evaluate the proposed framework.

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MS24

Use of Difference-Based Methods to Determine Statistical Models in Inverse Problems

We propose the use of difference-based methods with pseudo measurement errors to determine directly from data (without IP calculations and residual plots) an appropriate statistical model and then to subsequently investigate whether there is a mathematical model misspecification or discrepancy. In the presence of mathematical model misspecification, we also propose to use the information provided by pseudo measurement errors to quantify uncertainty in parameter estimation by bootstrapping methods.

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MS24

Estimation of Covariance Matrices in Ensemble Kalman Filtering

This talk discusses efficient implementations of the ensemble Kalman filter (EnKF) based on on shrinkage covariance estimation and on modified Cholesky decomposition. The proposed EnKF implementations exploit the conditional correlations of model components in order to obtain sparse estimators of the background error covariance matrix or its inverse. The forecast ensemble members at each step are used to estimate the background error covariance matrix via the Rao-Blackwell Ledoit and Wolf estimator, which has been specifically developed to approximate high-dimensional covariance matrices using a small number of samples. The estimation of inverse background error covariance is performed via the modified Cholesky decomposition. Different implementations are proposed in order to face typical scenarios in operational data assimilation. Numerical results are presented to illustrate how these estimates of background error correlations can increase the accuracy of EnKF analyses.

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MS24

The Intrinsic Dimension of Importance Sampling

We study importance sampling and particle filters in high dimensions and link the collapse of importance sampling to results about absolute continuity of measures in Hilbert spaces and the notion of effective dimension.

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MS24

A Limited Memory Multiple Shooting Approach for Weakly Constrained Data Assimilation

We present a variational limited memory method for state estimation of hidden Markov models. Our method is based on a multiple shooting approach that improves stability and a recursion to enforce optimality. The matching of states at checkpoints are imposed as constraints of the optimization problem which is solved with augmented Lagrangian method. We prove that for nonlinear systems within certain regime, the condition number of the augmented Lagrangian function is bounded above with respect to number of shooting intervals. Hence the method is stable for increasing time horizon. We demonstrate numerically the improved stability with Burgers' equation.

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MS25

Prediction Uncertainty for Solute Transport in Fractured Rock: From Theory to Experiments

Predictive modelling of solute transport in consolidated materials (rocks) is relevant in various engineering applications, from water supply to ecological risk assessment, from construction to waste disposal. Although basic processes are for the most part well understood, heterogeneity over the entire range of scales still poses a major challenge for predictive modelling. We present the theoretical basis for transport modelling and illustrate basic sensitivities to controlling mechanisms. Prediction uncertainty is computed for generic cases and then verified with experimental field data for three different configurations which combine inverse and forward modelling. The experiments selected are from the nuclear waste disposal programs in Sweden carried out as part of crystalline rock site investigations. It is shown that tracer transport can be predicted with reasonable confidence provided that the underlying physical mechanisms are well understood and suitably parametrized. We also present various strategies and open issues for improving confidence in predictive modelling of solute transport in fractured rock.

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MS25

Preliminary Analysis of Sampling Methods with Geological Prior Models for Solving Inverse Problems

In hydrogeology, the characterization of reservoirs by physical parameters (e.g. hydraulic conductivity, porosity, etc.) is required to understand and predict groundwater behavior. Inverse problems consists in identifying the parameter fields allowing to reproduce field observations of state variables. In general, this constitutes an ill-posed problem. Whereas optimization techniques (e.g. maximum likelihood methods) show very good performance when assuming that the parameter fields can be modeled using Gaussian processes, sampling methods are needed for a reasonable uncertainty quantification in the posterior space if a more general prior model is used. In this work, we consider prior models that are generated with Multiple Point Statistics (MPS). MPS is a non parametric approach allowing to generate realistic geological fields reproducing spatial features present in a training data set and honouring conditioning data. To sample the posterior space, MPS simulations are integrated in an iterative approach that consists in selecting suitable hard conditioning data at specific locations. We show that this approach is promising and accelerate the rate of convergence.

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MS25

Data Dimension Reduction for Seismic Inversion

Abstract not available.

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MS25

Determining the Mechanisms That Result in Hydraulic Fracturing Production Decline Using Inverse Methods and Uncertainty Quantification

Abstract not available.

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MS26

Impact of Spectral Sampling Techniques on Surrogate Modeling

Many science and engineering application explore high-dimensional parameter spaces by creating initial random samplings to build surrogate models. However, it is unclear how the sampling properties of this sample impact regression performance. We generalize spectral sampling techniques to high-dimensions, introduce a novel sample synthesis algorithm and present systematic comparisons with classical techniques. Preliminary results show that approaches, such as, Latin Hypercube designs produce significantly inferior samplings, i.e. require more points to produce equivalent regression errors.

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MS26

Experimental Design-based Methods for Simulating Probability Distributions

In this talk, I will explain an experimental design-based method for simulating complex probability distributions. The method requires fewer evaluations of the probability distribution and therefore, it has an advantage over the usual Monte Carlo or Markov chain Monte Carlo methods when the distribution is expensive to evaluate. I will explain the application of the proposed method in Bayesian computational problems, optimization, and uncertainty quantification.

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MS26

Kennedy-O'Hagan Model with Calibration Parameters: Parameter Identifiability, Estimation Consistency and Efficiency

Abstract not available.

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MS26

An Empirical Interpolation Method for a Class of Quasilinear PDEs with Random Input Data

We aim at approximating a class of quasi-linear parameterized PDEs by solving the corresponding SDEs with reduced-basis methods. The empirical interpolation method is utilized in our numerical schemes for SDEs to obtain the off-line online cost decomposition. The main feature of the SDE approach is that we do not need to solve linear or nonlinear systems when using implicit time-stepping schemes, leading to a significantly reduction by avoiding approximating the Jacobian of the nonlinear operator.

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MS27

Error Bounds for Regularized Least-squares Regression on Finite-dimensional Function Spaces

We present a framework to deduce bounds on the error of least-squares regression methods with smoothness constraints on finite-dimensional spaces. To this end, we rely on certain Jackson- and Bernstein-type inequalities in these spaces. We point out similarities and differences to the results in the infinite-dimensional setting, e.g. [Cucker & Zhou 2007], and results in the finite-dimensional setting without additional smoothness constraints, e.g. [Chkifa et al. 2015]. Finally, we apply our results to a sparse grid-based regression algorithm.

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MS27

Sparse Polynomial Chaos Expansions Via Weighted L1-Minimization

This talk is concerned with the solution of PDEs with random inputs where the solution-dependent quantity of interest (QOI) admits a sparse polynomial chaos (PC) expansion. As an extension of the standard l1-minimization, a widely used method for sparse approximation, we consider a weighted l1-minimization that relies on a priori knowledge on the PC coefficients to improve the solution recovery. We present theoretical and empirical results to demonstrate different aspects of this sparse approximation technique.

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MS27

Estimate of the Lebesgue Constant of Weighted Leja Sequence on Unbounded Domain

The Leja points are a sequence of nested interpolation points in one dimension, which show promise as a foundation for high-dimensional approximation methods. For the problem of weighted interpolation on the real line, we analyze the Lebesgue constant for a sequence of weighted Leja points. As in the unweighted case of interpolation on a bounded domain, we use results from potential theory to show that the Lebesgue constant for the Leja points grows subexponentially.

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MS27

Quasi-Optimal Points Selection for Radial Basis Function Interpolation and Its Application to UQ

Radial basis functions (RBF) provide powerful meshfree methods for multivariate interpolation for scattered data. The approximation quality and stability depend on the distribution of the center set. The optimal placements of the centers in the RBFs method are always unclear. In this talk, we present an efficient data-independent algorithm to select the distribution of centers. We then apply the method to parametric uncertainty quantification. Various numerical tests are provided to examine the performance of the methods.

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MS28

Weakly Intrusive Low-rank Methods for Model Order Reduction

A strategy is proposed for computing a low-rank approximation of a nonlinear parameter-dependent equation. For an iteration of a Newton algorithm, the residual and the preconditioner are approximated with weakly intrusive variants of the empirical interpolation method. The increment is then computed with a greedy rank-one algorithm, and the iterate is compressed in low-rank format. The efficiency of the proposed algorithm is illustrated with numerical examples.

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MS28

Joint Model and Parameter Dimension Reduction for Bayesian Inversion Applied to An Ice Sheet Problem

We consider Bayesian inference for ice sheet inverse problems, where exploration of the posterior suffers from the twin difficulties of high dimensionality of the uncertain parameters and computationally expensive forward models. We present a data-informed approach that jointly identifies intrinsic dimensionality in both parameter space and state space by exploiting the interplay between noisy observations and the physical model. We show that using only a limited number of model simulations, the resulting subspaces lead to an efficient method to explore the high-dimensional posterior.

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MS28

Rom for Uq Control Problems

We focus on reduced order modelling adaptive techniques to deal with UQ problems in the optimal control framework. A special focus is on multi-level sampling for greedy algorithm, combined with sparse-grid sampling. Approximation stability is discussed as well. Examples are taken from viscous flows.

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MS28

Projection Based Model Order Reduction for the Estimation of Vector-valued Variable of Interest

We present a projection-based model order reduction method for the estimation of vector-valued (or functional-valued) variables of interest associated to parameter-dependent equations. We first present an extension of the standard primal-dual approach. Then, we propose a new projection method based on a saddle-point problem which involves three reduced spaces: the approximation and test spaces associated to the primal variable, and the approximation space associated to the dual variable. In the spirit of the Reduced Basis method, we propose greedy algorithms for the construction of these reduced spaces.

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MS29

Explicit Cost Bounds of Stochastic Galerkin Approximations for Parameterized Pdes with Random Coefficients

We will present explicit bounds on the overall computational complexity of the stochastic Galerkin finite element method (SGFEM) for approximating the solution of parameterized elliptic partial differential equations with both affine and non-affine random coefficients. These bounds account for the sparsity of the SGFEM system that results from an orthogonal expansion of the random coefficient. We also present computational evidence complementing our theoretical estimates and a comparison with the stochastic collocation finite element method.

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MS29

Balanced Iterative Solvers for Linear Systems Arising from Finite Element Approximation of PDEs

This talk discusses the design of efficient solution algorithms for symmetric and nonsymmetric linear systems associated with FEM approximation of PDEs. The novel feature of our preconditioned MINRES and GMRES solvers incorporates error control in the natural norm (associated with the specific approximation space) in combination with a reliable and efficient a posteriori estimator for the PDE approximation error. Balancing the algebraic and the approximation error leads to a robust and balanced inbuilt stopping criterion.

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MS29

Hydrodynamic Stability and UQ

This talk highlights some recent developments in the design of robust solution methods for the Navier–Stokes equations modelling incompressible fluid flow. Our focus is on uncertainty quantification. We discuss stochastic collocation approximation of critical eigenvalues of the linearised operator associated with the transition from steady flow in a channel to vortex shedding behind an obstacle. Our computational results confirm that classical linear stability analysis is an effective way of assessing the stability of such a flow.

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MS29

Solving Log-Transformed Random Diffusion Problems by Stochastic Galerkin Mixed Finite Element Methods

We study mixed formulations of second-order elliptic problems where the diffusion coefficient is the exponential of a random field. We build on the previous work [E. Ullmann, H. C. Elman, O. G. Ernst, SIAM J. Sci. Comput., 34] and reformulate the PDE as a first-order system in which the logarithm of the diffusion coefficient appears on the left-hand side. This gives a sparse, but non-symmetric Galerkin matrix. We discuss block triangular and block diagonal preconditioners for the Galerkin matrix and analyze a practical approximation to its Schur complement.

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MS30

Non Parametric Calibration of Lvy Processes Via Kolmogorov's Forward and Backward Equation

We present an optimal control approach to the problem of model calibration for Lévy processes based on a non parametric estimation procedure. The calibration problem is of considerable interest in mathematical finance and beyond. Calibration of Lévy processes is particularly challenging as the jump distribution is given by an arbitrary Lévy measure, which form a infinite dimensional space. In this work, we follow an approach which is related to the maximum likelihood theory of sieves. The sampling of the Lévy process is modelled as independent observations of the stochastic process at some terminal time T. We use a generic spline discretization of the Lévy jump measure and select an adequate size of the spline basis using the Akaike Information Criterion (AIC). The numerical solution of the Lévy calibration problem requires efficient optimization of the log likelihood functional in high dimensional parameter spaces. We provide this by the optimal control of Kolmogorov's forward equation for the probability density function (Fokker-Planck equation). The first order optimality conditions are derived based on the Lagrange multiplier technique in a functional space. The resulting Partial Integral-Differential Equations (PIDE) are discretized, numerically solved and controlled using scheme a composed of Chang-Cooper, BDF2 and direct quadrature methods. The talk is based on joint work with Mario Annunziato

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MS30

Shape Optimization for Quadratic Functionals and States with Random Right-Hand Sides

In this talk, we investigate a particular class of shape optimization problems under uncertainties on the input parameters. More precisely, we are interested in the minimization of the expectation of a quadratic objective in a situation where the state function depends linearly on a random input parameter. This framework covers important objectives such as tracking-type functionals for elliptic second order partial differential equations and the compliance in linear elasticity. We show that the robust objective and its gradient are completely and explicitly determined by low-order moments of the random input. We then derive a cheap, deterministic algorithm to minimize this objective and present model cases in structural optimization.

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MS30

Shape Optimization with Uncertain Data

Since shapes are optimized typically only once and used later on frequently and in many unforeseen circumstance, uncertainty quantification is a high importance in the field of shape optimization. This talk discusses numerical aspects mainly in the practical application of aerodynamic shape optimization under uncertain loads and uncertainties with respect to the shape itself.

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MS31

Uncertainty Quantification for Multiscale Systems Using Deep Gaussian Processes

We present a novel approach for uncertainty quantification in multiscale models using deep Gaussian processes. Deep GPs are suitable for deep learning in high-dimensional complex systems consisting of several hidden layers connected with non-linear mappings. The dimensionality reduction technique required to develop this model is based on the Gaussian process latent variable model which provides a flexible technique for non-linear dimensionality reduction. The method is applied to a number of stochastic multiscale PDE problems.

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MS31

Model Error Quantification for High-Dimensional Bayesian Inverse Problems

While a parametric fit can almost always be achieved with various model calibration tools, if the underlying model is incorrect, it will lead to erroneous predictions. The traditional approach of using an additional regression model (e.g. GPs) to account for model errors is practically infeasible in high-dimensions, can violate physical constraints and does not provide the requisite insight. In this work, conservation & constitutive laws are unfolded and probabilistic estimates for model discrepancies are computed.

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MS31

Sequential Monte Carlo in Truly High-dimensional Models

It is widely believed that for sequential Monte Carlo methods to work in high-dimensional models the effective dimensionality of the system needs to be low. Against this belief, we will discuss a class of local algorithms that can exploit decay of correlations in truly high-dimensional models and yield error bounds that are uniform both in time and space.

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MS31

On the Low Dimensional Structure of Bayesian Inference via Measure Transport

A recent approach to non-Gaussian Bayesian inference seeks a deterministic transport map that pushes forward a reference density to the posterior. In this talk, we address the computation of transport maps in high dimensions. In particular, we show how the Markov structure of the posterior density induces low-dimensional parameterizations of the transport map. Topics include the sparsity of inverse triangular transports, the ordering of the Knothe-Rosenblatt rearrangement, decompositions of transports, and other related ideas in dimensionality reduction for Bayesian inversion.

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MS32

Quantifying the Effect of Parameter Uncertainties on the Simulation of Drought in the Community Atmosphere Model

We analyze a perturbed physics ensemble performed with the Community Atmospheric Model to gain insights into causes of the 1998-2002 North American drought. The ensemble was constructed by varying the values of input parameters related to physical parameterizations over allowable ranges of uncertainty. We perform a sensitivity analysis to identify the key parameters influencing drought-related metrics. We also identify parameter values that yield a better fit to data, resulting in a better simulation of drought.

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MS32

Estimation of the Coefficients in a Coulomb Friction Boundary Condition for Ice Sheet Sliding on Bedrocks

When modeling the sliding of ice sheets over a solid bedrock, one of the most difficult aspects is the treatment of the boundary condition at the ice-bedrock interface. In this presentation we consider a regularized Coulomb sliding condition, where the friction coefficient depends on the ice velocity. Our focus will be on the estimation of the parameters in the sliding condition, with the goal of finding a general and portable expression for the friction coefficient.

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MS32

Emulation of Future Climate Uncertainties Arising from Uncertain Parametrizations

The Whole Atmosphere Community Climate Model (WACCM) is a comprehensive numerical model. Many parameterizations of physical processes have to be set, resulting in potential concerns about error growth. To assess future climate uncertainties, we need to develop statistical models that can reproduce the outputs, and retrieve the uncertainties about the parameters and outputs in past and present climates. We perform uncertainty analysis and the emulation by calibrating the gravity waves parameters and accelerating the algorithm.

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MS32

Uncertainty Quantification for NASA's Orbiting Carbon Observatory 2 (OCO-2) Mission

OCO-2 measurements of atmospheric carbon dioxide are inferred from observed radiance spectra. The inference uses Bayes' Theorem: a "retrieval" algorithm computes the posterior mean and covariance matrix of atmospheric state vectors given the radiances. However, there are additional sources of uncertainty including computational artifacts and uncertain algorithm parameters. Here we describe our approach to quantifying these uncertainties in aggregate in order to provide more realistic characterizations of atmospheric CO2 globally.

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MS33

A Multi-Order Monte Carlo Discontinuous Galerkin Method for Wave Equations with Uncertainty

We show how recently developed arbitrary order accurate (in space and time) discontinuous Galerkin methods for wave equations in second order form can be used to design multi-order Monte Carlo methods. We compare the complexity to the multilevel Monte Carlo approach as well as to methods that are fixed order in time and arbitrary order in space. We also present experiments illustrating the properties of the method.

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MS33

Numerical Methods for Stochastic Conservation Laws

Stochastic conservation laws (SCL) provides a connection between conservation laws and Hamilton–Jacobi equations and are used in models of mean field games. An impressive collection of theoretical results has been developed for SCL in the recent years. In this talk we present numerical methods for strong and weak solutions of SCL with Gaussian randomness in rough fluxes and forcing terms.

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MS33

Multilevel Monte Carlo Approximation of Statistical Solutions of Incompressible Flow

We present a finite difference-(Multi-level) Monte Carlo algorithm to efficiently compute statistical solutions of the two dimensional Navier-Stokes equations, with periodic boundary conditions and for arbitrarily high Reynolds number. We propose a reformulation of statistical solutions in the vorticity-stream function form. The vorticity-stream function formulation is discretized with a finite difference scheme. We obtain a convergence rate error estimate for this approximation. We also prove convergence and complexity estimates, for the (Multi-level) Monte Carlo finite-difference algorithm to compute statistical solutions. Numerical experiments illustrating the validity of our estimates are presented. They show that the Multi-level Monte Carlo algorithm significantly accelerates the computation of statistical solutions, even for very high Reynolds numbers. Supported by ERC StG NN 306279 SPARCCLE (to S. Mishra), and by the Swiss National Supercomputing Centre CSCS Grant s590

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MS33

A Sparse Stochastic Collocation Technique for High Frequency Wave Propagation with Uncertainty

We consider the wave equation with highly oscillatory initial data, where there is uncertainty in the wave speed, initial phase and/or initial amplitude. To estimate quantities of interest related to the solution and their statistics, we combine a high-frequency method based on Gaussian beams with sparse stochastic collocation. Although the wave solution, u^ε, is highly oscillatory in both physical and stochastic spaces, we provide theoretical arguments and numerical evidence that quantities of interest based on local averages of $|u^\varepsilon|^2$ are smooth, with derivatives in the stochastic space uniformly bounded in ε, where ε denotes the short wavelength. This observable related regularity makes the sparse stochastic collocation approach more efficient than Monte Carlo methods. We present numerical tests that demonstrate this advantage.

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MS34

A Bayesian Level-Set Approach for Geometric In-

verse Problems

We introduce a Bayesian level-set approach for PDE-constrained inverse problems where the unknown is a geometric feature of the underlying PDE forward model. By means of state-of-the-art MCMC methods we describe numerical experiments that explore the posterior distribution that arises from (i) inverse source detection (ii) the identification of geologic structures in groundwater flow (iii) the estimation of electric conductivity in the complete electrode model for EIT.

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MS34

Reversible Proposal Mcmc in High Dimension

Metropolis-Hastings (MH) algorithm with reversible proposal transition kernel includes many useful MCMC algorithms such as random-walk Metropolis, independent type MH and pCN algorithms. These MCMC algorithms are easy to design, free from gradient calculation and are easy to incorporate statistical information. In this talk, we analyse high dimensional asymptotic property of those methods, especially for heavy tailed target distribution. Also, we discuss the application to statistical inference for high dimensional stochastic diffusion models.

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MS34

Adaptive Random Scan Gibbs Samplers

Is the uniform coordinate choice optimal for the Random Scan Gibbs Sampler? I will present an adaptive Random Scan Gibbs Sampler that guided by approximating the optimal L^2 convergence on a Gaussian target improves on the uniform selection probabilities directing computational effort towards difficult coordinates. The improvement will be illustrated on computational examples and ergodicity of this non-markovian adaptive MCMC algorithm will be discussed.

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MS34

Title Not Available

Abstract not available.

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MS35

Artificial Boundary Conditions and Domain Truncation in Electrical Impedance Tomography

Electrical impedance tomography (EIT) is an imaging modality in which unknown conductivity distribution is reconstructed from surface voltage measurements. The solution is based on mathematical model (the complete electrode model) which comprises of the diffusion equation and related boundary conditions. In principle, the accurate solution of the problem would require that the boundary conditions such as currents through the boundaries of the computational domain are known. In practice this would mean that all currents through the boundary should happen only on the electrodes. However, in some applications, such as in geological imaging, this would require the computational domain to be very large and the computational problem can be exceedingly heavy. In this work we consider an approach which allows truncation of the computational domain without significant loss in the accuracy of the solution due to unknown boundary conditions (boundary data). We formulate the truncated p roblem using so called Dirichlet-to-Neumann (DtN) map, which connects the voltages on the artificial boundary to the current flows through the boundary. In the inverse problem, the DtN map is treated as a unknown random quantity which is estimated from measurements along with the conductivity distribution. This is possible due to a low-dimensional parametrization of DtN map using PCA basis. This is joint work with J.P. Kaipio, P. Hadwin D. Calvetti, and E. Somersalo.

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MS35

Iterative Ensemble Smoothers for Calibration and Uncertainty Quantification of Large Petroleum Reservoir Models

In this talk, I will describe some characteristics of the petroleum history matching problem that make characterization of uncertainty difficult. In particular, I will comment on the prior distribution on model variables, characteristics of the data, and typical calibration parameters. Iterative ensemble smoothers have been developed for solving these high-dimensional problems, and application will be shown.

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MS35

Polynomial Chaos Based Bayesian Identification Procedures

The need to identify the descriptive parameteric elements of some model by comparison with measurement is mostly resolved in a Bayesian framework with the help of computational algorithms based on sampling approaches. The goal of this work is to present a new kind of Bayesian estimate through a sampling-free method based on the spectral representations. In this way the low-rank approximation procedures can be easily used for the reduction of the computational time of posterior.

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MS35

Shape Uncertainty Quantification for Scattering Transmission Problems

The aim is to quantify how uncertain shape variations affect the optical response of a nano-device to some electromagnetic excitation. The 2D Helmholtz transmission problem for a particle in air is considered. We model the shape using a high-dimensional parameter, and adopt a domain mapping approach to obtain a variational formulation on a parameter-independent configuration. We present results obtained with high-order quadrature methods, and discuss nonsmooth parameter dependence cases, where only low-order methods (MLMC) converge.

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MS36

Sensitivity Analysis of Pulse Wave Propagation in Human Arterial Network

The effect of uncertainties on the pulse wave propagation in the human one-dimensional arterial network is investgated. The uncertainties are either issued from the cardiac output or from local parameters in the network like the arterial stifness of given arteries (the aorta for instance). The study is based on the use of a stochastic sparse pseudospectral method and expresses the sensitivity of the solution with relevant factors such as pulse pressure at various locations.

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MS36

Posterior Adaptation of Polynomial Surrogate for Bayesian Inference in Arterial Flow Networks

Bayesian inference is a robust but costly framework for solving hemodynamic inverse problem, i.e., inferring mechanical properties and parameters of an arterial system from simulated and measured blood pressure and flow. We propose to adaptively construct a polynomial surrogate that focuses accuracy over the targeted parametric region of interest. The method is tested on the inference of vessel properties in reduced models of pulse waves in arterial networks with measurements from actual patients.

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MS36

Assimilation and Propagation of Clinical Data Uncertainty in Cardiovascular Modeling

Availability, consistency and variability of clinical measurements affect the predictive performance of cardiovascular models, suggesting the need to include such uncertainty in data assimilation practices. Starting from an analysis of the structural and practical, local and global parameter identifiability in 0D circulation models with applications in pediatric and adult diseases monitoring, we combine multi-level Bayesian estimation, adaptive MCMC and multi-resolution uncertainty propagation to lean model parameters and quantify confidence in numerical predictions.

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MS36

Integrating Clinical Data Uncertainty in Cardiac Model Personalisation

For patient-specific models of the heart to translate into clinical decisions, a measure of confidence in their predictions is needed. This requires moving from deterministic approaches to probabilistic ones, with challenges both methodologically, as deriving stochastic models of such complex phenomena is difficult, and computationally, as such approaches are much more demanding. I will present methods using uncertainty quantification and machine learning in order to integrate data uncertainty in clinical applications of cardiac models.

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MS37

On Dynamic Nearest-Neighbor Gaussian Process Models for High-Dimensional Spatiotemporal Datasets

With the growing capabilities of Geographic Information Systems (GIS) and user-friendly software, statisticians today routinely encounter geographically referenced data containing observations from a large number of spatial locations and time points. Over the last decade, hierarchical spatial-temporal process models have become widely deployed statistical tools for researchers to better understanding the complex nature of spatial and temporal variability. However, fitting hierarchical spatial-temporal models often involves expensive matrix computations with complexity increasing in cubic order for the number of spatial locations and temporal points. This renders such models unfeasible for large data sets. In this talk, I will present two approaches for constructing well-defined spatial-temporal stochastic processes that accrue substantial computational savings. Both these processes can be used as "priors" for spatial-temporal random fields. The first approach constructs a low-rank process operating on a lower-dimensional subspace. The second approach constructs a Nearest-Neighbor Gaussian Process (NNGP) that can be exploited as a dimension-reducing prior embedded within a rich and flexible hierarchical modeling framework to deliver exact Bayesian inference. Both these approaches lead to Markov chain Monte Carlo algorithms with floating point operations (flops) that are linear in the number of spatial locations (per iteration). We compare these methods and demonstrate its use in inferring on the spatial-temporal distribution of ambient air pollution in continental Europe using spatial-temporal regression models with chemistry transport models.

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MS37

Modelling Extremes on River Networks

Max-stable processes are the natural extension of the classical extreme-value distributions to the functional setting, and they are increasingly widely used to estimate probabilities of complex extreme events. In this talk I shall discuss how to broaden them from the usual setting in which dependence varies according to functions of Euclidean distance to the situation in which extreme river discharges at two locations on a river network may be dependent, either because the locations are flow-connected or because of common meteorological events. In the former case dependence depends on river distance, and in the second it depends on the hydrological distance between the locations, either of which may be very different from their Euclidean distance. Inference for the model parameters is performed using a multivariate threshold likelihood, which is shown by simulation to work well. The ideas are illustrated with data from the upper Danube basin. The work is joint with Peiman Asadi and Sebastian Engelke.

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MS37

Investigating Nested Geographic Structure in Consumer Purchases: A Bayesian Dynamic Multi-Scale Spatiotemporal Modeling Approach

Abstract not available.

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MS37

Predictive Model Assessment in Spatio-temporal Models for Infectious Disease Spread

Routine public health surveillance of notifiable infectious diseases gives rise to daily or weekly counts of reported cases stratified by region, age group and possibly gender. Probabilistic forecasts of infectious disease spread are central for outbreak prediction, but need to take into account temporal dependencies inherent to communicable diseases, spatial dynamics through human travel and social contact patterns between age groups and gender. We describe a multivariate time series model for weekly surveillance counts on noroviral gastroenteritis from the 12 city districts of Berlin in five age groups from 2011 to 2014. Spatial dispersal is captured by a power-law formulation based on the order of adjacency between districts while social contact data from the POLYMOD study was used to describe disease spread between age groups. Calibration and sharpness of the probabilistic one-step-ahead and long-term forecasts obtained with this model are assessed using proper scoring rules.

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MS38

Quantifying Uncertainty in the Prediction of Pollutant Dispersion

The transport of pollutants in urban environments is influenced by turbulent wind flows that are governed by the large-scale variability of the atmospheric boundary layer. To improve the predictive capabilities of CFD simulations of pollutant dispersion, the uncertainty related to this variability and to the turbulence model should be quantified. In this talk we will propose a framework to achieve this goal and present results obtained for simulations of the Joint Urban 2003 field experiment.

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MS38

Physics-Derived Model Form Uncertainty in Turbulent Combustion

The major challenge in turbulent combustion modeling is the sheer number of models that are invoked, each of which involves its own set of assumptions and subsequent model error. In this work, two methods are presented for deriving model errors directly from physics: hierarchical models and peer models. Hierarchical models use a high-fidelity model to estimate the uncertainty in a lower-fidelity model, and peer models use models with differing assumptions to derive an uncertainty estimate.

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MS38

Bayesian Optimal Experimental Design for Estimating Parameters of Turbulence Models

Velocity and Reynolds stress sensor configurations extracting the most useful information for estimating the turbulence model parameters in flow models are obtained by optimizing an expected utility associated with either the information entropy or the Kullback-Leibler divergence. Bayesian asymptotic approximations simplify drastically the computational burden due to excessive number of flow model simulations. Stochastic optimization algorithms such as the CMA-ES are necessary to avoid premature convergence to local optimal.

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MS38

Preliminary Study of a Stochastic Rans Model Exploiting Local Model Inadequacy Indicators

The lack of an universal RANS model creates the need for quantifying local modeling uncertainty to assess the reliability of a simulation without experimental validation data. In this contribution, we apply state-of-the-art methods for local error detection (Gorl et al., 2011; Ling and Templeton, 2015) based on physical reasoning and machine learning algorithms for the estimation of local failure of a RANS turbulence model. This information is then used to stochastically perturb the model locally.

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MS39

Methods for Electronics Problems with Uncertain Parameters: An Overview

In electronic engineering applications, the variability of parameters has to be included into the design cycle to achieve reliable products. We focus on the modeling of uncertainties by random variables or random processes. An overview is given on the relevant problems as well as methods. The numerical techniques are based on sampling methods, stochastic collocation schemes or a stochastic Galerkin approach. We identify challenges in modeling and simulation to quantify uncertainties for electronics industry.

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MS39

Stochastic Inverse Problem of Material Parameter Reconstruction in a Passive Semiconductor Structure

We focus on the reconstruction of material parameters under uncertainties in a model of a passive semiconductor device. For the UQ propagation in a 3D model, governed by Maxwell's equations, the Spectral Collocation Method (SCM) is used. The inverse problem deals with the identification of real-functions aiming to reduce iteratively a random-dependent regularized cost functional that consists of the weighted mean and standard deviation values. The gradient directions are computed using the Adjoint Variable Method and Tellegen's theorem combined with the SCM. Simulations involving the reconstruction based on measurements are performed, showing the robustness and efficiency of the proposed algorithm.

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MS39

Efficient Evaluation of Bond Wire Fusing Probabilities

Integrated circuits are often connected to their packaging using bond wires. During operation the system can heat up, leading to a fusing of the wires. The probability of fusing (failure) in the presence of manufacturing imperfections is computed using surrogate based sampling techniques available in the literature. Both numerical results and a convergence analysis for the scheme are provided in the context of a coupled electrothermal simulation of the device.

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MS39

Parametric Model Order Reduction for Efficient Uncertainty Quantification of Nanoelectronic Devices

In robust design of nanoelectronic devices, uncertainty quantification (UQ) is indispensable. However, UQ for large-scale dynamical systems is computationally expensive: e.g., a non-intrusive method requires simulating the large-scale system at various parameter values. Therefore, parametric model order reduction (PMOR), which can efficiently build a small-scale model that is accurate on a specified parameter range, serves as a powerful tool for acceleration. Numerical results for several nanoelectronic devices validate the efficiency of PMOR for UQ.

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MS40

Inverse Modeling of Geochemical and Mechanical Compaction in Sedimentary Basins Through Polynomial Chaos Expansion

We illustrate a procedure to perform an uncertainty analysis for overpressure development in sedimentary basins. We consider compaction and fluid flow in stratified sedimentary basins subject to mechanical and geochemical processes. We perform (i) model reduction based on a generalized Polynomial Chaos Expansion (gPCE), (ii) maximum likelihood calibration of model parameters. We discuss the impact of availability of different types of data, e.g., pressure or porosity distributions, on parameter estimation results.

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MS40

Towards Geological Realism in Predicting Uncertainty in Reservoir Inverse Modelling: Geostatistics and Machine Learning

Use of informative priors in inverse reservoir modelling results in more accurate prediction of uncertainty based only

on geologically realistic models, which are consistent with the prior knowledge and initial assumptions about the geological interpretation. Proper geological priors in form of multi-dimensional parameter relations are elicited from natural analogue information using a machine learning approach. Furthermore, use of machine learning in geomodelling can facilitate integration of key reservoir uncertainties, such as multiple geological interpretation and relevant spatial scale representations.

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MS40

Stochastic Identification of Contaminant Sources

When a contaminant is detected at a drinking well, its source could be uncertain. We propose a stochastic technique to identify when and where such a contamination entered the aquifer, with a quantification of the uncertainty associated to such identification.

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MS40

Accounting for Known Sources of Model Error During Bayesian Posterior Sampling of Geophysical Inverse Problems

A methodology is presented to account for model errors resulting from inaccurate forward process representations in Bayesian solutions to near-surface geophysical inverse problems. We show how principal components analysis combined with an informal likelihood function based on the L2 norm can be used within MCMC to account for realistic model error in the corresponding posterior samples. We show the application of the method to ground-penetrating radar monitoring of infiltration to estimate unsaturated hydraulic properties.

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MS41

MUQ (MIT Uncertainty Quantification): A Flexible Software Framework for Algorithms and Applications

MUQ has many capabilities for defining and solving forward and inverse uncertainty quantification problems. In this talk, we will focus on our Markov chain Monte Carlo (MCMC) module and how appropriate software abstractions can accelerate MCMC algorithm development and testing. We then illustrate MUQs capabilities by creating a new surrogate-exploiting transport-map MCMC algorithm and solving a prototypical Bayesian inverse problem. We conclude by discussing how these extensible and reusable software frameworks facilitate reproducible science.

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MS41

UQTk: a C++/Python Toolkit for Uncertainty Quantification

The UQ Toolkit (UQTk) is a collection of libraries, tools and apps for the quantification of uncertainty in numerical 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 key UQTk capabilities and illustrate a typical UQ workflow.

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MS41

Opencossan: A Open Matlab Tool for Dealing with Randomness, Imprecision and Vagueness

OpenCossan is a open and collaborative software for uncertainty quantification and management. OpenCossan aims to promote learning and understanding of non-deterministic analysis through the distribution of an intuitive, flexible, powerful and open computational toolbox. Released under the LGPL license, OpenCossan can be used, modified and freely redistributed. The quantification of uncertainties and risks is a key requirement and challenge across various disciplines in order to operate systems of diverse nature safely under the changing state of inputs and boundary conditions. Randomness is represented mathematically by random quantities and by suitable probability distributions. However, many of the uncertain phenomena are non-repeatable events and the understanding in the underlying physics can also be limited or vague. A key feature of the software is its capability to deal with different representation of the uncertainty adopting concepts of Imprecise probability. This allows a rational treatment of the information of possibly different forms without ignoring significant information, and without introducing unwarranted assumptions. This software implements efficient simulation and parallelization strategies allowing a significant reduction of the computation costs of the non-deterministic analyses.

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MS41

Adaptive Sparse Grids for UQ with 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 input-modeling / model calibration via density estimation. We will show both use cases for a benchmark problem in CO2 storage. We demonstrate the use of the multi-platform sparse grid toolkit SG^{++}, which provides efficient implementations of adaptive sparse grids in different flavors.

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MS42

Sample-Efficient, Basis-Adaptive Polynomial Chaos Approximation

Methods for computing accurate approximations of a Quantity of Interest (QoI) via Polynomial Chaos and l1-regression with low-coherence sampling have developed promising numerical and theoretical results. We present an iterative method which for each iteration identifies a basis set and corresponding coefficients which adapt to the QoI as a function. Further, previously generated low-coherence samples are adapted for computations with subsequent bases by generating samples accounting for coherence adjustments arising from considering iteratively adapting bases.

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MS42

A Dictionary Learning Strategy for Bayesian Inference

To reduce the cost of evaluating the posterior in Bayesian inference, polynomial surrogates are typically used. We introduce a novel approach which does not rely on an a priori choice of basis for approximating the parameter field. From a prior set of realizations of the parameter field, one seeks a basis (dictionary) such that each realization is likely to admit a sparse representation. As demonstrated with our example, this approach can then accommodate scarce observations.

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MS42

Sparse Approximation Using L1-L2 Minimization

We propose a sparse approximation method using $\ell 1 - \ell 2$ minimization. We present several theoretical estimates regarding its recoverability for both sparse and non-sparse signals. Then we apply the method to sparse orthogonal polynomial approximations for stochastic collocation. Various numerical examples are presented to verify the theoretical findings. We observe that the $\ell 1 - \ell 2$ minimization seems to produce results that are consistently better than the $\ell 1$ minimization.

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MS42

Interpolation Via Weighted L1 Minimization

Abstract not available.

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MS43

The Probability Density Evolution Method for Multi-Dimensional Nonlinear Stochastic Dynamical Systems

The multi-dimensional nonlinear stochastic dynamical systems are encountered in various scientific and engineering disciplines. For instance, in earthquake engineering and wind engineering, engineering structures themselves or the attached energy dissipation subsystems may exhibit strong nonlinear behaviors under severe earthquakes or strong winds. Besides, randomness may occur in both structural parameters and excitations (inputs). Generally, great challenges exist in the analysis of such systems because: (1) these systems are multi-dimensional systems with large degrees of freedom in the order of magnitude of hundreds or even millions, but on the other hand, they are nonlinear systems, and thus could not be reduced or decomposed, say by the modal superposition method; (2) the randomness is involved and coupled with the nonlinearity, which leads to coupled problems either in the level of moments (e.g., the closure problem) or probability densities (e.g., the coupled multi-dimensional FPK equation for white noise excitations); and (3) the randomness involved might be non-stationary and non-Gaussian. In the present paper the probability density evolution method will be outlined. In this method, the principle of preservation of probability is invoked to tackle the system by explicitly introducing the sources of randomness and the embedded physics/dynamics mechanism. A state-variable decoupled generalized density evolution equation is then established. In contrast to the classical equations such as the FPK equation, this equation could be in any arbitrary dimensions rather in the dimension identical to the original dynamical system. Numerical methods will be discussed. A nonlinear structure subjected to seismic excitations will be studied.

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MS43

Uncertainty Propagation Across Distinct Pdf Systems and Stochastic Spectral Methods

Propagation of uncertainty across heterogeneous stochastic systems is an important research area that arises often in multi-fidelity modeling. The stochastic models can be classified from PDF models that contain the full statistical description of the stochastic solution, to surrogate models that provide the moments of the solution up to certain order. In this talk, we propose interface methods between these distinct stochastic systems, in particular, concerning the response-excitation PDF system. While this approach generalizes the classical PDF models to consider non-Gaussian colored noise, it involves the extended solution space from the excitation. We employ PDF transformation techniques to impose the boundary condition between classical and response-excitation PDF systems. In addition, we couple the PDF to stochastic spectral models by representing the random boundary in terms of orthogonal polynomial basis according to the probability measure provided from the PDF system. The effectiveness of our approach is demonstrated in stochastic advection-reaction equation.

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MS43

Method of Distributions for Uncertainty Quantification

Methods of distributions designate a class of approaches based on the derivation of deterministic partial differential equations for either a probability density function or a cumulative distribution function of a state variable. In this talk, we will discuss the mathematical foundation of such approaches as well as promises and limitations. Several applications will be discussed.

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MS43

Probabilistic Solutions to Random Differential Equations under Colored Excitation Using the Response-Excitation Approach

Equations for the evolution of the Response-Excitation (RE) pdf of non-Markovian responses of non-linear random differential equations (RDEs) under colored excitation are non-closed in general or exhibit limitations due to high-dimensionality. We present a closure scheme for the generalized RE Liouville equation (Athanassoulis, Tsantili, Kapelonis, 2015, Proc. R. Soc. A.,Vol. 471, p.20150501) for the long-time limit state of a scalar RDE that collects missing information through local linearized versions of the nonlinear RDEs.

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MS44

Set Oriented Numerical Methods for Uncertainty Analysis

In this talk we will introduce a numerical method which allows to perform a global uncertainty analysis for dynamical systems. The corresponding *uncertainty attractors* are computed by a sequence of nested, increasingly refined outer approximations. Thus, the numerical approach is inherently set oriented and therefore the method does not rely on long term simulations of the underlying system.

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MS44

Admm for 2-Stage Stochastic Quadratic Programs

We present a scenario-decomposition based Alternating Direction Method of Multipliers (ADMM) algorithm for the solution of scenario-based 2-stage stochastic Quadratic Programs. The decomposition alternates between: (i) an equality constrained quadratic program that is decoupled by scenarios and (ii) a projection onto a set bounds and the non-anticipativity constraints. We show that the projection problem scales linearly in the number of scenarios. Further, the decomposition allows using different values of the parameter for each of the scenarios. We provide convergence analysis and derive the optimal parameter setting for the ADMM parameter in each scenario. We show that the proposed approach outperforms the non-decomposed ADMM approach and compares favorably with Gurobi, a commercial QP solver, on a number test problems.

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MS44

A Chaotic Dynamical System That Samples

In this work, we construct a chaotic dynamical system that samples user prescribed distributions. This dynamical system is chaotic in the sense that although the trajectories are sensitive to initial conditions, but yet the same statistical properties are recovered every time the system is simulated (independent of the initial conditions). Combining ideas from ergodic theory and control theory, we construct a novel approach for building chaotic dynamical systems with predetermined statistical properties. On complicated distributions, we demonstrate that this algorithm provides significant acceleration and higher accuracy than competing methods (such as Hamiltonian MC, slice sampling and Metropolis-Hastings) for Markov Chain Monte Carlo (MCMC).We also demonstrate our novel algorithm by reproducing paintings and photographs, by treating them as the target distribution. If one makes the spatial distribution of colors in the picture the desired distribution, akin to a human, the algorithm first captures large scale features and then goes on to refine small scale features. The equations are easy to construct and can be simulated using standard Euler or Runge-Kutta integration schemes.

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MS44

Koopman Operator Based Nonlinear Estimation

We describe a new approach for observer design for nonlinear systems based on Koopman operator theoretic framework. Koopman operator is a linear but an infinite-dimensional operator that governs the time evolution of system outputs in a linear fashion. We exploit this property to synthesize an observer form which enables the use of Luenberger/Kalman-like linear observers for nonlinear estimation. We describe a numerical procedure to construct such an observer form and demonstrate it on several examples.

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MS45

Mild Stochastic Calculus in Infinite Dimensions

This talk presents a certain class of stochastic processes, which we suggest to call mild Ito processes, and a new, somehow mild, Ito type formula for such processes. We will use the mild Ito formula to establish essentially sharp weak convergence rates for numerical approximations of different types of stochastic partial differential equations including nonlinear stochastic heat equations, stochastic Burgers equations, stochastic Cahn-Hilliard-Cook type equations, and stochastic Wave equations.

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MS45

Numerical Approximation of Stochastic Differential Equations

In this talk we review some recent results on the numerical approximation of stochastic differential equations. We primarily focus on the mean-square error and show optimal convergence rates for the backward Euler-Maruyama method under a global monotonicity condition. Then we discuss some extensions of our results to the BDF2-Maruyama two-step scheme as well as to stochastic partial differential equations.

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MS45

SPDEs with Lévy Noise and Weak Convergence

In this talk, I will present an abstract framework to study the weak convergence of numerical approximations of linear stochastic partial differential equations of evolutionary type driven by additive Lévy noise. The central result is a general representation formula for the error, which is applied to study space-time discretizations of the stochastic heat equation, the wave equation, and a Volterra-type integro-differential equation as examples. For twice continuously differentiable test functions with bounded second derivative (with an additional condition on the second derivative for the wave equation) the weak rate of convergence is found to be twice the strong rate. The talk is based on joint work with Mihály Kovács and René Schilling.

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MS45

Computations of Waves in a Neural Model

Abstract not available.

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MS46

Scalable Parameterized Surrogates Based on Low Rank Tensor Approximations for Large-Scale Bayesian Inverse Problems

Hessian operators (of the negative log posterior) have played an important role in high-(infinite-) dimensional Bayesian inverse problems, from characterizing the (inverse of the) posterior covariance under the Gaussian approximation, to accelerating MCMC sampling methods by providing information on the local curvature in parameter space. The key to making computations with them tractable is a low rank approximation of the (prior-preconditioned) data misfit component of the Hessian. Here we consider the role of higher derivative operators in Bayesian inverse problems and whether scalable low rank approximations can be constructed.

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MS46

Accelerating MCMC with Active Subspaces

Active subspaces are an emerging set of tools for dimension reduction. When applied to MCMC, the active subspace separates a low-dimensional subspace that is informed by the data from its orthogonal complement that is constrained by the prior. With this information, one can run the sequential MCMC on the active variables while sampling independently according to the prior on the inactive variables.

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MS46

Subspace Acceleration Strategies for Sampling on Function Space

Many inference problems require exploring the posterior distribution of high-dimensional parameters, which in principle can be described as functions. Sampling posteriors defined on function space poses a significant challenge. By identifying and blending the global and local geometries informed by noisy observations, we present a suit of subspace accelerated schemes to tackle this challenge. Examples in a nonlinear inverse problem and a conditioned diffusion process are used to demonstrate the efficiency of our sampling schemes.

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MS46

Efficient Computations for Large-Scale Inverse Problems with Bayesian Sampling

The U.S. Department of Energy certifies weapons through modeling and simulation, which is informed by the results of experimentation wherein the results are delivered to the physics modelers with statistically valid estimates of uncertainty. While Bayesian sampling techniques are widely used for quantifying such uncertainty on signal and image reconstruction, they are computationally prohibitive in large--scale applications. We extend these approaches by implementing Monte Carlo schemes and matrix--free linear system solvers for reconstructions at the very large--scales, and demonstrate their viability on applications in quantitative radiographic data analysis.

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MS47

Bayesian Parameter Inference Across Scales

In multi-scale models, representations at different scales may depend on parameters that are not directly related. We propose a Bayesian approach for estimating fine scale parameters from the solution of the inverse problem at a coarser scale. Computed examples illustrate the viability of the approach.

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MS47

Bayesian Sampling Using a Wishart Prior in Radiography Image Reconstruction

Quantitative X-ray radiography hinges on the ability to solve inverse problems and provide uncertainties for image reconstructions. The Bayesian framework naturally lends itself to quantifying uncertainties and we have developed a hierarchical Bayesian method where we place a Wishart distribution on the prior precision matrix to provide enhanced edge information. This allows the data to drive the localization of features in the reconstruction. In this work we focus on Abel inversion to compute volumetric object densities from X-ray radiographs and to quantify uncertainties in the reconstruction. Results are presented for both synthetic signals and real data from a U.S. Department of Energy X-ray imaging facility.

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MS47

Expectation Propagation for Electrical Impedance Tomography

Electrical impedance tomography is a noninvasive imaging technique for determining the internal conductivity distribution from boundary voltage measurements. In this talk, we discuss a variational approach for electrical impedance tomography based on expectation propagation, which at each iteration involves numerical quadrature. Some numerical results for real data will be presented.

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MS47

Prior and Posterior Convergence for Some Finite Element Approximations

Finite element methods (FEM) are powerful tools for numerical approximations of partial differential equation. The rigorous mathematical background of FEM arises from thorough convergence studies. We will discuss applying the well-known convergence studies for FEM's within Bayesian statistical inverse problems, especially in the case of electrical impedance tomography.

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MS48

Multilevel Monte Carlo for Convective Transport in Inhomogeneous Media

In the last few years efficient algorithms have been proposed for the propagation of uncertainties through numerical codes. Recently, the multi-level Monte Carlo method emerged as a novel technique able to retain the robustness of the Montecarlo method, but increasing also its efficiency. We study the performance of the MLMC approach in simulation of particle-laden turbulent flow subject to thermal radiation. We also investigate strategies to further accelerate the approach using variance reduction techniques.

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MS48

Fast Bayesian Optimal Experimental Design for Seismic Source Inversion

We develop a fast method for optimally designing experiments in the context of statistical seismic source inversion. In particular, we efficiently compute the optimal number and locations of the receivers or seismographs. The seismic source is modeled by a point moment tensor multiplied by a time-dependent function. The parameters include the source location, moment tensor components, and start time and frequency in the time function. The forward problem is modeled by elastodynamic wave equations. We show that the Hessian of the cost functional, which is usually defined as the square of the weighted L2 norm of the difference between the experimental data and the simulated data, is proportional to the measurement time and the number of receivers. Consequently, the posterior distribution of the parameters, in a Bayesian setting, concentrates around the "true" parameters, and we can employ Laplace approximation and speed up the estimation of the expected Kullback- Leibler divergence (expected information gain), the optimality criterion in the experimental design procedure. Since the source parameters span several magnitudes, we use a scaling matrix for efficient control of the conditional number of the original Hessian matrix.

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MS48

Computing Measure Valued and Statistical Solutions of Hyperbolic Systems of Conservation Laws

We consider UQ for nonlinear hyperbolic systems of conservation laws within the frameworks of measure valued and statistical solutions and present a novel algorithm to compute these solutions. The algorithm, based on sampling and ensemble averaging, is shown to converge provided that the underlying space-time discretizations satisfy certain criteria. We show convergence of interesting observables such as moments, correlations, structure functions and multi-point statistics. Numerical experiments demonstrating the validity of this framework for unstable and turbulent flows are presented. More efficient variants such as MLMC methods and a coarse-graining algorithm are also considered.

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MS48

Continuation Multi Level Monte Carlo for Uncertainty Quantification in Compressible Aerodynamics

The aim of this work is to address the challenge of efficiently propagating geometrical and operating uncertainties in compressible aerodynamics numerical simulations with a Continuation Multi Level Monte Carlo algorithm. We will present numerical test case (nozzle and the RAE2822 airfoil) of interest in compressible aerodynamics and show the efficiency of the proposed CMLMC in terms of accuracy versus overall computational cost, compared to a standard MC method and its robustness on these applications.

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MS49

A Piecewise Deterministic Markov Process for Efficient Sampling in R^n

In recent work (Bierkens, Roberts 2015) we discovered an elementary piecewise deterministic Markov process (zig zag process) which can be extended to have a general (absolutely continuous) invariant probability distribution in R^n. We develop MCMC based on the zig zag process. The sample paths of the zig zag process can be efficiently simulated by rejection sampling of the switching times. We compare the resulting algorithm to other important sampling methods. It turns out that the zig zag process is particularly efficient at sampling from heavy tailed probability distributions.

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MS49

Improving the Performance of Overdamped Langevin Samplers by Breaking Detailed Balance

MCMC provides a powerful and general approach for generating samples from a high-dimensional target probability distribution, known up to a normalizing constant. There are infinitely many Markov processes whose invariant measure equals a given target distribution. The natural question is whether a Markov process can be chosen to generate samples of the target distribution as efficiently as possible. It has been previously observed that adding an appropriate nonreversible perturbation to a reversible Markov process will improve its performance. In this talk, I will describe some recent results which characterise the effect of adding a nonreversible drift to an overdamped Langevin sampler, in terms of rate of convergence to equilibrium and asymptotic variance. Finally, I will detail how such nonreversible Langevin samplers can be used in practice by describing a discretisation scheme which inherits the good performance of the underlying process.

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MS49

The Backward Sde Filter

A novel adaptive meshfree forward backward doubly stochastic differential equation approach is presented for the nonlinear filtering problem. The algorithm is based on the fact that the solution is the unnormalized filtering density required in the nonlinear filtering problem. Adaptive space points are constructed in a stochastic manner to improve the efficiency of the algorithm. We also present numerical results for (i) a double well potential problem with oscillations and (ii) a multi-target tracking problem.

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MS49

Gibbs-Langevin Samplers

Abstract not available.

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MS50

Empirical Bayes Approach to Climate Model Calibration

One challenge for Bayesian calibration of climate models is the question of how to assign weights to various observational targets, many of which are highly correlated through the physics of the atmosphere. We will discuss the use of 'hyper-parameters' and how they can be enhanced by additional information from a set of perfect modeling experiments in order to provide an indication of the significance of gaps between a model and observations.

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MS50

Greater Accuracy with Reduced Precision: A Stochastic Paradigm for Weather and Climate Prediction

Weather and climate models have become increasingly important tools for making society more resilient to extremes of weather and for helping society plan for possible changes in future climate. These models are based on known laws of physics, but, because of computing constraints, are solved over a considerably reduced range of scales than are described in the mathematical expression of these laws. This generically leads to systematic errors when models are compared with observations. A new paradigm is proposed for solving these equations which sacrifices precision and determinism for small-scale motions. It is suggested that this sacrifice may allow the truncation scale of weather and climate models to extend down to cloud scales in the coming years, leading to more accurate predictions of future weather and climate

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MS50

Probabilistic Regional Ocean Predictions

This presentation is concerned with the prediction of the probability distribution function (pdf) of large nonlinear dynamical systems using stochastic partial differential equations (S-PDEs), with a focus on regional ocean dynamics. The stochastic dynamically orthogonal (DO) PDEs for a primitive equation ocean model with nonlinear free surface are derived and numerical schemes for their space-time integration are obtained. Examples are provided for a set of idealized multiscale non-hydrostatic and hydrostatic flows as well as for more realistic regional ocean dynamics. Results are compared to more classic ensemble approaches. Such comparisons utilize stochastic predictive skill metrics developed for real-time ocean pdf forecasts issued with the Error Subspace Statistical Estimation (ESSE) method during Aug-Sep 2009 for the two-month QPE IOP09 experiment off the coast of Taiwan.

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MS50

A Parametrization of Ocean Mesoscale Eddies: Stochasticity and Non-viscous Stresses

Ocean mesoscale eddies strongly affect the strength and variability of large-scale flows. Parametrizing eddy-mean flow processes in climate simulations remains a key challenge, especially quantifying the uncertainty associated with parametrized eddies. We show that a successful closure for turbulent mesoscale eddies can be obtained using resolved non-Newtonian stresses. The uncertainty associated with the parametrization can be quantified using a stochastic model which depends only the coarse resolution, wind stress and stratification.

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MS51

Tensor Train Approximation of the First Moment Equation for Elliptic Problems with Lognormal Coefficients

We study the elliptic equation with coefficient modeled as lognormal random field. A perturbation approach is adopted, expanding the solution in Taylor series. The resulting recursive deterministic problem satisfied by the expected value of the solution (first moment equation) is discretized with full tensor product finite elements. We develop an algorithm for solving the recursive high dimensional first moment equation in a low-rank format (Tensor Train) and show its effectiveness with numerical examples.

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MS51

Blending Finite Dimensional Manifold Samplers

with Dimension-Independent MCMC

Bayesian inverse problems involve sampling probability distributions on functions. Traditional MCMC algorithms fail under mesh-refinement. Recently, a variety of dimension-independent MCMC methods have emerged, but few of them take the geometry of the posterior into account. In this work, we blend finite dimensional manifold samplers with dimension-independent MCMC to enjoy the benefit of geometry, whilst remaining robust under mesh-refinement. The key idea is to employ the manifold methods on an appropriately chosen finite dimensional subspace.

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MS51

Dynamical Low Rank Approximation of Incompressible Navier Stokes Equations with Random Parameters

We investigate the Dynamically Orthogonal approximation of time dependent incompressible Navier Stokes equations with random parameters. The approximate solution is sought in the low dimensional manifold of functions with fixed rank, written in separable form, and it is obtained by performing a Galerkin projection of the governing equations onto the time-dependent tangent space of the approximation manifold along the solution trajectory. Numerical tests at moderate Reynold number will be presented, with emphasis on the case of stochastic boundary conditions.

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MS51

Solution of Stochastic PDEs Via Low-Rank Separated Representation: A Randomized Alternating Least Squares Approach

Finding solutions, in separated form, to stochastic PDEs via fixed point iteration requires a reduction algorithm, typically alternating least squares (ALS), to reduce the separation rank after each iteration. Conditioning of least squares matrices in ALS iterations affects the convergence of fixed point iterations. We propose a randomized variation of ALS to improve conditioning. Our numerical examples illustrate how better conditioning improves the performance of the fixed point iteration.

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MS52

Functional Car Models for Large Spatially Correlated Functional Datasets

Abstract not available.

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MS52

Tukey g-and-h Random Fields

We propose a new class of trans-Gaussian random fields named Tukey g-and-h (TGH) random fields to model non-Gaussian spatial data. The proposed TGH random fields have extremely flexible marginal distributions, possibly skewed and/or heavy-tailed, and, therefore, have a wide range of applications. The special formulation of the TGH random field enables an automatic search for the most suitable transformation for the dataset of interest while estimating model parameters. An efficient estimation procedure, based on maximum approximated likelihood, is proposed and an extreme spatial outlier detection algorithm is formulated. The probabilistic properties of the TGH random fields, such as second-order moments, are investigated. Kriging and probabilistic prediction with TGH random fields are developed along with prediction confidence intervals. The predictive performance of TGH random fields is demonstrated through extensive simulation studies and an application to a dataset of total precipitation in the south east of the United States. The talk is based on joint work with Ganggang Xu.

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MS52

Fusing Multiple Existing Space-Time Land Cover Products

The assessment, monitoring, and characterization of land cover (LC) is essential for global change research as it is a critical variable driving many environmental processes. Most efforts have focused either on improving the accuracy of LC products from remote sensing data or on the assimilation and synthesis of existing LC datasets using statistical interpolation techniques.We develop a methodology for fusing multiple existing LC products to produce a single LC record over a long time period and a large spatial domain. We must first reconcile the thematic map classifications of the different LC products and then interpolate LC in space and time on a specified domain. Our probabilistic interpolation approach includes a direct estimation of the uncertainty associated with the spatio-temporal prediction of LC, and we provide an illustration using six LC products over the Rocky Mountain region of the United States.

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MS52

Testing for Spatial and Spatio-Temporal Stationarity

Abstract not available.

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MS53

Uncertainty in Massflow Measurements in Pipes Due to Bends

The dominant source of uncertainty in flow-rate measurements in pipes (with e.g. ultrasonic flow meters) is the lack of knowledge of the true velocity profile. In particular a relatively narrow spectrum of velocity profiles can appear downstream of a bend. This study aims at quantifying the uncertainty in massflow measurements due to bends and design sensor locations, and multi-sensor systems that minimize this uncertainty.

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MS53

Surrogate-Based Robust Airfoil Optimization Considering Geometrical Uncertainties

We will present surrogate-based robust shape optimization of transonic airfoils. A large number of geometrical uncertainties on the airfoil is modeled by a truncated Karhunen-Love expansion to achieve a dramatic reduction of the large number of parameters. The combination of quasi Monte Carlo sampling and gradient-enhanced Kriging enables us to efficiently calculate statistics of the aerodynamic coefficients which are used to evaluate the objective function to be optimized in our robust design optimization framework.

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MS53

An Investigation of Uncertainty Effects in Mixed Hyperbolic- Parabolic Problems Due to Stochastically Varying Geometry

We study mixed hyperbolic parabolic problems with uncertain stochastically varying geometries. The numerical solution is computed using a finite difference formulation on summation-by-parts form with weak boundary conditions. We prove that the continuous problem is well posed and that the semi-discrete problem is stable. The statistics are computed non-intrusively using quadrature rules given by the probability density function of the random variable. Numerical calculations are performed and the statistical properties of the solution are discussed.

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MS53

Robust Design Optimization of a Supersonic Natural Laminar Flow Wing-Body

A robust aerodynamic shape design problem related to an aerodynamic configuration of a supersonic business jet wing-body is here illustrated. The baseline configuration was designed within the SUPERTRAC EU project, and the aim of the present work is to improve the robustness and reliability of the baseline in presence of perturbations and uncertainties in operating conditions and in wing shape. The robust optimization approach adopted is based on the usage of value-at-risk and conditional value-at-risk.

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MS54

Causality Or Correlation? Multiscale Inference and An Application to Geoscience

One of the challenges in analysis of multiscale processes is to learn about the causality relations in the considered systems on a certain level of resolution - and to distinguish between the true causality from simple statistical correlations. Proper inference of such causality relations, besides giving an additional insight into such processes, can allow improving the respective mathematical and computational models. However, inferring such relations directly from equations/models is hampered by the multiscale character of the underlying processes and the presence of latent/unresolved/subgrid scales. Implications of missing/unresolved scales for this problem will be discussed and an overview of methods for data-driven causality inference will be given. Recently-introduced data-driven multi scale causality inference framework for Boolean data will be explained and illustrated on analysis of historical climate teleconnection series and on inference of their mutual influences on a monthly scale. It will be also shown how the obtained causality networks can be used for the network-driven regularization of the ill-posed data analysis problems for noisy data.

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MS54

Rigorous Intermittency in Turbulent Diffusion

Models with a Mean Gradient

Intermittency of passive tracer can be described as large spikes randomly occurring in the time sequence or exponential like fat tails in the probability density function. This type of intermittency is subtle and occurs without any positive Lyapunov exponents in the system. By exploiting an intrinsic conditional Gaussian structure, the enormous fluctuation in conditional variance of the passive tracer is found to be the source of intermittency in these models. An intuitive physical interpretation of such enormous fluctuation can be described through the random resonance between Fourier modes of the turbulent velocity field and the passive tracer. This intuition can be rigorously proved in a long time slow varying limit, where the limiting distribution of the passive tracer is computed through an integral formula.

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MS54

A Probabilistic Decomposition-Synthesis Method for the Quantification of Rare Events

We consider the problem of probabilistic quantification of dynamical systems that have heavy-tailed characteristics. These heavy-tailed features are associated with rare transient responses due to the occurrence of internal instabilities. Systems with these characteristics can be found in a variety of areas including mechanics, fluids, and waves. Here we develop a computational method, a probabilistic decomposition-synthesis technique, that takes into account the nature of internal instabilities to inexpensively determine the non-Gaussian probability density function for a quantity of interest. Our approach relies on the decomposition of the statistics into a non-extreme core, typically Gaussian, and a heavy-tailed component. We demonstrate the probabilistic decomposition-synthesis method for rare events in two dynamical systems exhibiting extreme events: a two-degree-of-freedom system of nonlinearly coupled oscillators, and in a nonlinear envelope equation characterizing the propagation of unidirectional water waves.

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MS54

Improving Prediction Skill of Imperfect Turbulent Models Through Statistical Response and Information Theory

A recent mathematical strategy for calibrating imperfect models in a training phase and accurately predicting the response by combining information theory and linear statistical response theory are developed in a systematic fashion for both full and reduced order models. A systematic hierarchy of simple statistical imperfect closure schemes are designed and tested which are built through new local and global statistical energy conservation principles combined with statistical equilibrium fidelity. As a further development, we use the stochastic models to predict intermittency in turbulent diffusion of passive tracer systems. Empirical information theory is used to measure the autocorrelation function under spectral representation. The optimal model improves the prediction skill uniformly in accurately capturing the crucial tracer statistical features.

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MS55

Making Uncertainty Quantification of Multi-Component Reactive Transport Manageable

Simulating multi-component (bio)reactive transport in the subsurface is computationally very expensive so that direct application of Monte-Carlo techniques for uncertainty quantification (UQ) is prohibitive. Linearized UQ is hampered by nonlinearity, but often the problems can be simplified by identifying conservative components, that are transported linearly, and restricting the reactions to primary controls. We present examples of estimating *pdf*s of reactive-constituents concentrations in heterogeneous media under conditions controlled by mixing or by electron-donor supply.

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MS55

Concentration Statistics for Transport in Heterogeneous Media: Self-Averaging, Mixing Models and the Evolution of Uncertainty

We study the PDF of concentration point values in heterogeneous porous media. We contrast the concentration PDFs obtained through spatial sampling and stochastic sampling, and discuss them in terms of the mean and mean squared concentrations. Specifically, we focus on the role of medium heterogeneity and the dynamics of mixing in the evolution of the concentration PDF, which we quantify in terms of the Lagrangian fluid deformation. We discuss mixing models that reflect these dynamics in an effective way and allow to quantify the evolution of the concentration PDF and thus concentration uncertainty. These properties depend on the mixing state of the system and the efficiency of local mass transfer properties in homogenizing the transport system. This has an impact also on the self-averaging properties of observables such as the effective dispersion coefficients.

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MS55

Subsurface Flow Simulations in Stochastic Discrete Fracture Networks

We focus on the Discrete Fracture Network model, in which the medium is modeled as a 3D set of intersecting polygons resembling fractures. Within this framework, we consider several sources of uncertainty, involving both the network geometry and hydrogeological properties (e.g., fracture transmissivities, orientation, dimensions...). We address the problem of quantifying the influence of these stochastic parameters on the output of DFN models, pursuing this target by applying modern UQ techniques to several stochastic configurations.

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MS55

Sparse Grid and Monte Carlo Methods for Groundwater Transport Problems

We focus on groundwater transport problems and consider arrival times related to particle trajectories subject to molecular diffusion and driven by a stochastic Darcy velocity obtained from log-normally distributed permeabilities. The goal is to efficiently compute statistics of such arrival times, e.g. their mean or the probability of exiting the physical domain in a given time horizon. We discuss several scenarios and propose both adaptive sparse grid stochastic collocation and Monte Carlo type schemes.

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MS56

Recent Advances in Dakota UQ

Sandia's Dakota software facilitates advanced exploration of simulations with various algorithms, including sensitivity analysis, optimization, and UQ. This presentation will survey Dakotas capabilities, interfaces, and algorithms. It will then highlight recent developments, including architecture improvements and algorithm R&D that aim to make uncertainty quantification practical for complex science and engineering models. Growth directions such as architecture modularity, graphical user interfaces, and improved algorithms for sensitivity analysis, surrogate modelling, and Bayesian inference, will be reviewed.

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MS56

The Parallel C++ Statistical Library Queso: Quantification of Uncertainty for Estimation, Simulation and Optimization

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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MS56

Handling Large-Scale Uncertainty Quantification with SmartUQ

Uncertainty quantification methods are widely used in engineering and science. However uncertainty quantification for large-scale problems poses great challenges. Through a combination of novel sampling and prediction techniques, several of these challenges have been overcome. An overview of these new techniques is presented along with examples of the application of UQ methods using these techniques as implemented in the SmartUQ software package.

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MS56

Chaospy: A Modular Implementation of Polynomial Chaos Expansions and Monte Carlo Methods

Chaospy is a Python toolbox specifically developed to implement polynomial chaos expansions and advanced Monte Carlo methods. The toolbox is highly modular with a programming syntax close to the mathematical theory. This talk will consists of an implementation walk-through with theoretical review and practical examples. The focus will be on (non-intrusive) methods where the software for the underlying model can be reused without modifications.

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MS57

Efficient Sampling Schemes for Recovering Sparse PCE

ℓ_1-minimization is an efficient technique for estimating the coefficients of a Polynomial Chaos Expansion (PCE) from a limited number of model simulations. In this talk I will present a generalized sampling and preconditioning scheme to accurately approximate high-dimensional models from limited data using any orthonormal PCE basis. The efficacy of this method will be demonstrated with various numerical and theoretical results.

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MS57

Germ-Transformed Polynomial Chaos Expansions

When confronted to configurations where the number of available code evaluations is low compared to the number of input variables, only low maximal polynomial order can be used, and the relevance of the associated polynomial chaos expansion (PCE) can be limited. To circumvent this problem, we propose, first, to transform the input variables by a parametrized function, and then, to carry out a PCE on these modified input variables.

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MS57

Mixing Auto-Regressive Models and Sparse Polynomial Chaos Expansions for Time-Variant Problems

Pure vanilla polynomial chaos expansions are known to fail at representing the time-varying output of computational models with random input parameters, especially in long time horizons. Such problems appear e.g. in earthquake engineering where the displacements history of a structure is of interest. In this talk we introduce autoregressive exogenous models (ARX) in conjunction with sparse polynomial chaos expansions to provide efficient time-dependent surrogates and we show their accuracy in selected applications.

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MS57

Iteration Method for Enhancing the Sparsity

The combination of generalized polynomial chaos (gPC) and compressive sensing is a useful tool for uncertainty quantification when the available data is limited. We propose a method to detect important subspaces through iterations, hence the sparsity of the representation of the system is enhanced. With this enhancement, the efficiency of the compressive sensing algorithm can be improved, and a more accurate gPC approximation is available. We use PDEs to demonstrate the efficiency of this method.

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MS58

Probabilistic Active Subspaces: Learning High-Dimensional Noisy Functions Without Gradients

We develop a probabilistic version of active subspaces (AS) which is gradient-free and robust to observational noise, relying on a novel Gaussian process regression with built-in dimensionality reduction. We demonstrate that our method is able to discover the same AS as the traditional gradient-based approach. The addendum of our approach is the determination of the dimensionality of the AS using Bayesian model selection. We use our model to propagate geometric/material uncertainties through high-dimensional granular crystals.

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MS58

Optimization Under Uncertainty of High-Dimensional, Sloppy Models

Optimization under uncertainty of high-dimensional, sloppy models This paper is concerned with the optimization of high-dimensional, complex models in the presence of uncertainty. This is hindered by the usual difficulties encountered in UQ tasks but also by the need to solve a nonlinear optimization problem involving large numbers of design variables We recast the problem as one of probabilistic inference and employ a Variational Bayesian (VB) formulation that also reveals a low-dimensional set of most sensitive directions in the design variable space.

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MS58

Recursive Cokriging Models for Global Sensitivity

Analysis of Multi-Fidelity Computer Codes

Complex computer codes are widely used in science and engineering to model physical phenomena. Global sensitivity analysis aims to identify the input parameters which have the most important impact on the code output. Sobol indices are a popular tool for performing such analysis. However, their estimates require an important number of simulations and often cannot be processed under reasonable time constraint. To handle this problem, we consider in this presentation the problem of building a fast-running approximation also called surrogate model of a complex computer code. The cokriging based surrogate model is a promising tool to build such an approximation when the complex computer code can be run at different levels of accuracy. We present here an original approach to perform a multifidelity cokriging model which is based on a recursive formulation. This approach allows to obtain original results. First, closed-form formulas for the universal cokriging predictive mean and variance can be derived. Second, it has a reduced computational complexity compared to the previous multifidelity models. This allows to easily provide Sobol index estimates by taking into account the metamodel error.

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MS58

Multi-Fidelity Information Fusion Algorithms for High Dimensional Systems and Massive Data-Sets

We construct response surfaces of complex deterministic and stochastic dynamical systems by blending variable information sources through Gaussian processes and autoregressive stochastic schemes. Hierarchical functional decompositions and local projections encode structure in GP priors, and enable the decomposition of the global learning problem into a series of low-dimensional tasks. These developments lead to linear complexity algorithms as demonstrated in benchmark problems involving deterministic and stochastic fields in up to 10^5 dimensions and 10^5 training points.

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MS59

Optimal L2-Norm Empirical Importance Weights for the Change of Probability Measure

We propose an optimization formulation to determine a set of empirical importance weights to achieve a change of probability measure, in the case of random samples generated from an unknown distribution. The importance weights associated with the random samples are computed such that they minimize the L2-norm between the weighted empirical distribution function and the desired distribution function. The resulting optimization problem is solved efficiently at scale. A variety of test cases are presented.

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MS59

Zero-variance Approaches in Static Reliability Problems

Computing reliability metrics on complex systems is done either considering stochastic processes modeling the evolution with time of the system, or taking a static view where the system and its components have a random but fixed state (the usual one being binary, either they work or they don't). The latter are sometimes called static models, because time is not an explicit parameter to deal with. Numerical evaluation of these metrics is hard or impossible in many cases, because of the model's size. Monte Carlo estimation is a possible solution, but then, the rare event problem strikes. For dealing with it, one of the most promising approaches today is the "zero-variance" idea, established when the model is a stochastic process. In this talk we show how to adapt the idea to a static setting, and we illustrate it with numerical results showing that it can be extremely powerful also for this class of models.

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MS59

From Probability-Boxes to Imprecise Failure Probabilities Using Meta-Models

A common situation in engineering practice is to have a small set of measurements which is insufficient to characterize a probabilistic model. Then probability-boxes provide a framework to describe the inherent uncertainty more adequately. The propagation of probability-boxes through a computational model, however, is computationally expensive and especially in the case of rare events may become intractable. The use of meta-models reduces the computational effort and allows for an efficient estimation of failure probabilities.

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MS59

Speeding Up Monte Carlo Simulations by Using An

Emulator

Monte Carlo simulations is used in integrated circuit design for yield optimization, statistical variability analysis and predicting failure probability. The Monte Carlo is time consuming but independent of the number of statistical parameters. Therefore, speedup is crucial and a new approach needed. We introduce an Emulator technique based on an accept and reject algorithm for accelerating the Monte Carlo simulations and getting a speedup 10x.

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MS60

$\mathcal{H}$-Matrix Accelerated Second Moment Analysis for Potentials with Rough Correlation

The efficient solution of operator equations with random right hand side is considered. The solutions two-point correlation is well understood if the two-point correlation of the right hand side is known and sufficiently smooth. Unfortunately, the problem becomes more involved in case of rough data. However, the rough data and also the inverse operators can efficiently be approximated by means of $\mathcal{H}$-matrices. This enables us to solve the problem in almost linear time.

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MS60

Lattice Test Systems for Qmc Integration

We discuss a number of lattice systems which are relevant for models in elementary particle physics. These systems can serve as benchmark models to test the feasibility of QMC and iterated numerical integration methods. In particular, it will be most interested to see, whether these methods can outperform standard MC techniques as presently used in particle physics computations.

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MS60

Very High Dimensional Integration Problems in Quantum Lattice Gauge Theory

We consider very high d-dimensional integration problems arising in the field of lattice gauge theory. The integration problems range from the scalar case (integration over $[0,1]^d$ or $\mathbb{R}^d$) to integration over the d-product of spheres or even the d-product of more complex manifolds like $SU(3)$. We report improvements over traditional MCMC methods for one dimensional physical systems with very high d, and present problems from general models in two and three physical dimensions.

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MS60

A Practical Multilevel Higher Order Quasi-Monte Carlo Method for Simulating Elliptic Pdes with Random Coefficients

We present a Multilevel Quasi-Monte Carlo method, based on rank-1 lattice rules, and demonstrate its performance for solving PDEs with random coefficients. We numerically show that the cost of the method is inversely proportional to the requested tolerance on the error. Next, we present the extension of the multilevel idea to higher order digital nets, and discuss the corresponding computational complexity.

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MS61

Several Visualization Issues in Uncertainty and Sensitivity Analysis of Model Outputs

While exploring a simulation computer code, one can be faced to the complexity of its input and/or output variables. For temporal or spatial phenomena, tools have to be adapted to the data functional and uncertain nature in order to understand and synthesize their behavior. We will illustrate several practical issues coming from various applications, as well as applications of new visualization methods. We will focus on the issue of uncertainty analysis and sensitivity analysis of model outputs.

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MS61

Functional Data Visualization: An Extension of the Highest Density Regions Boxplot

In this work, we propose a visualization method adapted from the Highest Density Region boxplot, a functional version of the boxplot. This tool is especially aimed at visualizing simultaneously multivariate functional data. It relies on the study of the coefficients of the data on the first few components of a decomposition basis. The plotted descriptive statistics are the so-called multivariate functional median, envelopes of the most central regions and outlying curves.

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MS61

Vizualizing the Uncertainty Represented by Vector-Valued Ensemble Fields

In this talk I will discuss visualization techniques for analysing the uncertainty that is represented by an ensemble of vector fields, to determine the major trends and outliers in the shape and spatial location of relevant field structures. I will focus on the problem of how to generate and visualize distributions for streamlines in vector fields, based on the clustering of similar shapes and by using visual abstractions for the streamlines distributions in these clusters.

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MS61

Analysis and Visualization of Ensembles of Shapes

The visualization of stochastic or uncertain data is typically referred to "uncertainty visualization". However, this terminology implies associated set of assumptions about the paradigm for visualization, which is typically to display an answer that has been modulated or augmented by an associated uncertainty. This however, asserts the existence of a renderable answer, which defies one of the underlying goals or principles of visualization, which is the exploration of data to obtain a holistic understanding or to discover properties that have no associated, a priori hypothesis. An alternative paradigm, is "variability visualization" where the goal of the visualization is to explore or better understand the set of possible outcomes, or the probability distribution, associated with a set of data. One example of such an approach is the method of contour boxplots, which relies on a generalization of data depth, from descriptive statistics, to render the variability of solutions in an ensemble of isocountours.

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MS62

Efficiently Computing Covariance of Parameter Estimates in Inverse Problems

Uncertainty quantification in inverse problems presents distinct opportunities and challenges relative to UQ in forward models. A formal solution for the *a posteriori* probability distribution (PPD) for inverse problems is often readily available, but is difficult to work with practically. For unimodal posteriors, the PPD may be approximately characterized by its mode and covariance about the mode. Computing these quantities can present formidable challenges. In practice, finding the MAP estimate may require minimizing a very high dimensional function ($O(10^5 - 10^6)$ parameters) with complex (e.g. discretized nonlinear) PDE constraints. For such a problem, merely storing the final covariance may require tens of terabytes. We show that the structure of inverse problems leads to a sparse update on a predictable and *a priori* known covariance operator. This leads to an efficient sparse basis in which to compute and store the covariance. We show how the covariance can be accurately computed with relatively little computation over and above that used in finding the MAP estimate. This method can thus be used to compute the uncertainty in an inverse problem solution relatively efficiently. We describe the approach formally in a relatively general setting, and demonstrate it with examples in inverse diffusion and inverse elasticity.

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MS62

Estimating Large-Scale Chaotic Dynamics

Obvious likelihood approaches are not available for chaotic systems, due to the sensitivity of the trajectories to any perturbations in the calculations. For large systems, such as used for weather predictions, Ensemble Prediction Systems (EPS) are used to quantify the uncertainty. Here we extend EPS, with essentially no additional CPU costs, to online estimation by perturbing the model parameters as well. The estimation can be performed both by a covariance update process using importance weights, or by employing evolutionary (DE) optimisation. Here we emphasize the use of DE for multiple cost function situations.

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MS62

Dynamic Mutual Information Fields and Adaptive Sampling

We present a novel methodology for predicting mutual information fields and for adaptive sampling in high-dimensional fields. The methodology exploits the governing nonlinear dynamics and captures the non-Gaussian structures. The spatially and temporally varying mutual information field in general nonlinear dynamical systems is efficiently quantified. Optimal observation locations are determined by maximizing the mutual information between the candidate observations and the variables of interest. The globally optimal sequence of future sampling locations is rigorously determined by dynamic programming approaches that combine mutual information fields with the predictions of the forward reachable set. All the results are exemplified and their performance is quantitatively assessed using a variety of simulated fluid and ocean flows.

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MS62

Convolved Hidden Markov Models applied to Geophysical Inversion

Consider a sequence of categorical facies classes along a subsurface well profile. Convolved geophysical observations are available. Focus is on assessing the categorical profile given geophysical observations. Bayesian inversion, with convolved likelihood and Markov chain prior is defined. The posterior is not easily assessable due to extensive coupling. An approximate k-factorial posterior is defined and exactly assessed by the extended forward-backward algorithm. The exact posterior is assessed by McMC sampling using this approximate posterior.

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MS63

A Tv-Gaussian Prior for Infinite Dimensional Bayesian Inverse Problems

Many scientific and engineering problems require to perform Bayesian inferences in function spaces, in which the unknowns are of infinite dimension. In such problems, choosing an appropriate prior distribution in these problem is an important task. In particular we consider problems where the function to infer is subject to sharp jumps which render the commonly used Gaussian measures unsuitable. On the other hand, the so-called total variation (TV) prior can only be defined in a finite dimensional setting, and does not lead to a well-defined posterior measure in function spaces. In this work we present a TV-Gaussian (TG) prior to address such problems, where the TV term is used to detect sharp jumps of the function, and the Gaussian distribution is used as a reference measure so that it results in a well-defined posterior measure in the function space. We also present an efficient Markov Chain Monte Carlo (MCMC) algorithm to draw samples from the posterior distribution of the TG prior. With numerical examples we demonstrate the performance of the TG prior and the efficiency of the proposed MCMC algorithm.

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MS63

High-Dimensional Bayesian Inversion with Priors Far from Gaussians

We discuss Bayesian inversion with priors that strongly deviate from a Gaussian structure, motivated by sparsity and edge preserving approaches in imaging. A major challenge is the highly anisotropic structure of the priors, which calls for evaluations with different measures than variance or mean square risks. We present some approaches based on Bregman risks, which also provide novel view points on MAP estimates. Moreover we comment on some pitfalls and the appropriate modelling of prior knowledge in such situations.

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MS63

Besov Space Priors and X-Ray Tomography

Consider an indirect measurement $m = Au + e$, where u is a function and e is random error. The inverse problems is "given m, find an approximation of u in a noise-robust way". In practical Bayesian inversion one models m, u and e as random variables and constructs a finite-dimensional computational model of the measurement. The data m is complemented with a priori information using Bayes formula. Approximate reconstructions of u can then be achieved as point estimates from the posterior distribution. Discretization-invariance means that if the computational model is refined, then the Bayesian estimates and probability distributions converge towards infinite-dimensional limiting objects. Computational examples are presented for demonstrating the properties of wavelet-based Besov space priors, which are the first non-Gaussian priors known to be discretization-invariant. Furthermore, we present a theoretical approach for resolving the white noise paradox appearing as the discretisation of the measurement is refined arbitrarily. Namely, realisations of infinite-dimensional white noise are square-integrable only with probability zero, which motivates a modification of the classical inversion approach.

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MS63

Efficient Bayesian Estimation Using Conditional Expectations

In this talk we will show a novel method of computing approximations to the mean square error estimator (MMSE),

which is equivalent to the conditional expectation and as such a kind of Bayesian estimator, and its use for assimilation of measured data into surrogate models of stochastic responses. The proposed method can be seen as a generalisation of the Kalman filter to general distributions and non-linear measurement operators. An application to the identification of the log-conductivity of a subsurface Darcy flow by measurements of a pollutant will be shown.

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MS64

Sparse Identification of Nonlinear Dynamics: Governing Equations from Data

Abstract not available.

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MS64

Low-Dimensional Modeling and Control of Nonlinear Dynamics Using Cluster Analysis

Abstract not available.

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MS64

Bayesian Inference of Biogeochemical-Physical Dynamical Models

Abstract not available.

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MS64

Structure and Resilience of Two-Dimensional Fluid Flow Networks

Abstract not available.

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MS65

Title Not Available

Abstract not available.

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MS65

Parallel Adaptive Importance Sampling

Abstract not available.

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MS65

Incremental Local Approximations for Computationally Intensive Mcmc on Targeted Marginals

We introduce approximate MCMC methods to characterize selected marginals of high-dimensional probability distributions, in a setting where density evaluations are computationally taxing. Our approach uses importance sampling to estimate the targeted marginal density, as in pseudo-marginal MCMC, but combines noisy estimates via local polynomial or GP approximations to capture the smooth underlying marginal density. The approach is incremental in that local approximations are refined as MCMC sampling proceeds, yielding an asymptotically exact low-dimensional chain

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MS65

Variance Estimation and Allocation in the Particle Filter

We introduce estimators of the variance and weakly consistent estimators of the asymptotic variance of particle filter approximations. These estimators are defined using only a single realization of a particle filter, and can therefore be used to report estimates of Monte Carlo error together with such approximations. We also provide weakly consistent estimators of individual terms appearing in the asymptotic variance, again using a single realization of a particle filter. When the number of particles in the particle filter is allowed to vary over time, the latter permits approximation of their asymptotically optimal allocation. Some of the estimators are unbiased, and hence generalize the i.i.d. sample variance to the non-i.i.d. particle filter setting.

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MS66

Polynomial Chaos-Based Bayesian Inference of K-Profile Parametrization in a General Circulation

Model of the Torpical Pacific

We present a Polynomial Chaos (PC)-based Bayesian inference method for quantifying the uncertainties of K-Profile Parametrization (KPP) model in MIT General Circulation Model (MITgcm). The inference of the uncertain parameters is based on a Markov Chain Monte Carlo (MCMC) scheme that utilizes a newly formulated test statistic taking into account the different components representing the structures of turbulent mixing on both daily and seasonal timescales in addition to the data quality, and filters for the effects of parameter perturbations over those due to changes in the wind. To avoid the prohibitive computational cost of integrating the MITgcm model at each MCMC iteration, we build a surrogate model for the test statistic using the PC method. The traditional spectral projection method for finding the PC coefficients suffered from convergence issues due to the internal noise in the model predictions. Instead, a Basis-Pursuit-DeNoising (BPDN) compressed sensing approach was employed that filtered out the noise and determined the PC coefficients of a representative surrogate model. The PC surrogate is then used to evaluate the test statistic in the MCMC step for sampling the posterior of the uncertain parameters. We present results of the posteriors that indicate a good agreement with the default values for two parameters of the KPP model namely the critical bulk and gradient Richardson; while the posteriors of the remaining parameters were hardly informative.

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MS66

Field Sensitivity Analysis of the Circulation in the Gulf of Mexico Using a PC Representation

A global sensitivity analysis is performed of the combined impact of uncertainties in initial conditions and wind forcing on the circulation in the Gulf of Mexico. To this end, polynomial chaos surrogates are constructed using a basis pursuit denoising methodology. The computations reveal that whereas local quantities of interest can exhibit complex behavior that necessitates a large number of realizations, the modal analysis of field sensitivities can be suitably achieved with a moderate size ensemble.

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MS66

Model Reduction for Climate Model Structural Uncertainty Quantification

A significant source of uncertainty in climate model predictions is the structural uncertainty arising from modeler choices in numerical approximations and parameterizations, which results in a multi-model ensemble approach to prediction. We examine the use of reduced models to emulate the behavior of more complex numerical simulations in order to efficiently explore the uncertainties arising from different model structures.

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MS66

Ensemble Variational Assimilation

Ensemble Variational Assimilation (EnsVAR) consists in perturbing the data to be assimilated according to their error probability distribution, and then perform variational assimilation on the perturbed data. EnsVAR achieves exact Bayesian estimation in the linear Gaussian case. EnsVAR is implemented on small-dimension chaotic systems. It achieves a high degree of bayesianity (as measured by statistical reliability). Its performance compares favourably with that of other ensemble assimilation algorithms, such as Ensemble Kalman Filter and Particle Filter.

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MS67

Exploiting Tensor Structure in Bayesian Inverse Problems

We discuss how to exploit low-rank tensor structure in high-dimensional inference and data assimilation problems, treated in a Bayesian setting. In particular, we show how one can utilize low-rank representations of the likelihood and dynamics to yield efficient representations of the posterior density. We also use a recently developed continuous extension to the tensor-train decomposition in order to obtain efficient sampling in areas of large posterior probability.

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MS67

Bayesian Inversion Using Hierarchical Tensor Approximations

Recovering equation parameters from real-world measurements is a challenging task that has raised interest in different areas of applied mathematics and engineering. When relying on Bayes' theorem, the high dimensionality of the involved integrals often are tackled by sampling methods which usually only exhibit slow convergence. We present a novel approach for Bayesian inversion which employs a recently developed efficient hierarchical tensor representation of the solution of the forward problem. In the talk, we outline the advantages of the employed TT-decomposition and present comparisons with some well-known methods.

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MS67

Spectral Likelihood Expansions and Nonparametric Posterior Surrogates

Abstract not available.

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MS67

Rapid Bayesian Inference on Bayesian Cyclic Networks

A new framework is developed for rapid Bayesian inference, involving probabilistic mappings between continuous and discrete data and model spaces on a quaternary Bayesian cyclic network. In this method, a continuous data space is mapped to a discrete data space (order reduction), and thence to a discrete model space (Bayesian updating). This is inverted to infer the continuous model space. The method facilitates rapid Bayesian inference for high-volume, real-time applications, including turbulent flow control.

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MS67

Stochastic Collocation Methods for Nonlinear Probabilistic Problems in Solid Mechanics

Abstract not available.

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MS68

Bayesian Models for Uncertainty Quantification of

Antarctic Ice Shelves

The challenges in quantifying uncertainty in ice modeling have their roots in the intricacy of the equations governing ice dynamics: so much computational power is required for the accurate simulation of coupled ice sheet/shelf complexes that only few model runs can be accomplished, which in turn renders the uncertainty sampling too sparse. We present a statistical approach with which current (hypothetical or former) ice shelves can be modeled and reconstructed. By combining spatial processes at various scales and approximations of break-off processes in a Bayesian hierarchical model we are able to quantify uncertainties of ice sheet processes within a straightforward simulation setting. We illustrate our approach with various contemporary Antarctic ice shelves.

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MS68

An Adaptive Spatial Model for Precipitation Data from Multiple Satellite over Large Regions

Satellite measurements have of late become an important source of information for climate features such as precipitation due to their near-global coverage. We look at a precipitation dataset during a 3-hour window over tropical South America that has information from two satellites. We develop a flexible hierarchical model to combine instantaneous rain rate measurements from those satellites while accounting for their potential heterogeneity. Conceptually, we envision an underlying precipitation surface that influences the observed rain as well as absence of it. The surface is specified using a mean function centered at a set of knot locations, to capture the local patterns in the rainrate, combined with a residual Gaussian process to account for global correlation across sites. To improve over the commonly used pre-fixed knot choices, an efficient reversible jump scheme is used to allow the number of such knots as well as the order and support of associated polynomial terms to be chosen adaptively. To facilitate computation over a large region, a reduced rank approximation for the parent Gaussian process is employed

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MS68

Full Scale Multi-Output Spatial Temporal Gaussian Process Emulator with Non-Seperable Auto-Covariance Function

Gaussian process emulator with separable covariance function has been utilized extensively in modeling large computer model outputs. The assumption of separability imposes constraints on the emulator and may negatively affect its performance in some applications where separability may not hold. We propose a multi-output Gaussian process emulator with a nonseparable auto-covariance function to avoid limitations of using separable emulators. In addition, to facilitate the computation of nonseparable emulator, we introduce a new computational method, referred to as the Full-Scale approximation method with block modulating function (FSA-Block) approach. The FSA-Block is an effective and accurate covariance approximation method to reduce computations for Gaussian process models, which applies to both nonseparable and partially separable covariance models. We illustrate the effectiveness of our method through simulation studies and compare it with emulators with separable covariances. We also apply our method to a real computer code of the carbon capture system.

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MS68

Fused Adaptive Lasso for Spatial and Temporal Quantile Function Estimation

Quantile functions are important in characterizing the entire probability distribution of a random variable, especially when the tail of a skewed distribution is of interest. This article introduces new quantile function estimators for spatial and temporal data with a fused adaptive Lasso penalty to accommodate the dependence in space and time. This method penalizes the difference among neighboring quantiles, hence it is desirable for applications with features ordered in time or space without replicated observations. The theoretical properties are investigated and the performance of the proposed methods are evaluated by simulations. The proposed method is applied to particulate matter (PM) data from the Community Multiscale Air Quality (CMAQ) model to characterize the upper quantiles, which are crucial for studying spatial association between PM concentrations and adverse human health effects.

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MS69

Innovative Methodologies for Robust Design Optimization with Large Number of Uncertainties

This paper describes the methodologies developed by ESTECO in UMRIDA Project and implemented in modeFRONTIER software. An adaptive regression methodology to reduce number of Polynomial Chaos terms is proposed for the Uncertainty Quantification. About Robust Design Optimization, a new approach is proposed, based on min-max definition of the objectives, and on the application of Polynomial Chaos for an accurate definition of percentiles (reliability-based robust design optimization). Aeronautical CFD test cases are proposed for validation.

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MS69

Manufacturing Tolerances in Industrial Turbo-Machinery Design

Abstract not available.

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MS69

Non-Adaptive Construction of Sparse Polynomial Surrogates in Computational Aerodynamics

A core ingredient for the construction of polynomial surrogates of complex systems is the choice of a dedicated sampling strategy, so as to define the most significant scenarii to be considered for the construction of such metamodels. Observing that system outputs may depend only weakly on the cross-interactions between the variable inputs, one may argue that only low-order polynomials significantly contribute to these surrogates. This feature prompts the use of reconstruction techniques benefiting from the sparsity of the outputs, such as compressed sensing. The results obtained with aerodynamic computations involving complex fluid flows corroborate this expected trend. In the mean time, we show how to compute arbitrary moments of orthogonal polynomials for the statistical analysis of the outputs from the surrogates. This research has received funding from the European Union's Seventh Framework Programme for research, technological development and demonstration under grant agreement no ACP3-GA-2013-60503.

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MS69

Efficient Usage of 2nd Order Sensitivity for Uncertainty Quantification

We propose a method based on nodal representation of geometrical uncertainty field. Such discretization leads to a large set of correlated uncertainties that is too big to be analyzed with existing methods in reasonable time. The proposed approach is based on the idea of reducing the number of analyzed uncertainties. In order to do this one needs to compute directional 2nd order derivatives. This approach is expected to give significant gain in computational time.

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MS70

Dynamic Patterns in the Brain

There is a broad need in neuroscience to understand and visualize large-scale recordings of neural activity, big data acquired by tens or hundreds of electrodes recording dynamic brain activity over minutes to hours. Such datasets are characterized by coherent patterns across both space and time, where many transient events are present at different temporal scales. I will talk about our work applying dynamic mode decomposition (DMD) to large-scale neural recordings. As a specific example, we combined spatio-temporal coherent patterns extracted by DMD with unsupervised machine learning to identify and characterize networks of sleep spindles. We uncovered several distinct sleep spindle networks identifiable by their stereotypical cortical distribution patterns, frequency, and duration.

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MS70

Multiscale Relations Measure for Categorical Data and Application to Genomics

Inference of relations between categorical data sets is an important problem in many areas of computational biology and bioinformatics. One of the essential problems hereby emerging - and frequently leading to strongly-biased and even completely wrong results and interpretations - is induced by the multiscale character of the biological systems, manifested in a presence of latent/unresolved variables, as well as in the issue of a model error - resulting from (may be wrong) a priori mathematical assumptions about the underlying processes. Combining tools and concepts from information theory with the exact law of the total probability, we derive a multiscale relation measure that - in terms of the underlying mathematical assumptions - is less restrictive and allows to infer an eventual impact from the latent variables. At the same time, it has a same leading order of the computational complexity (linear in the size of the data statistics) as the standard relation measures. Application of this measure to the analysis of single nucleotide polymorphisms (SNPs) in a part of the human genome reveals more complex relation patterns than implied by standard measures - thereby providing an indication that many of the interpretations deduced from the genomic data may be resulting from the bias induced by too restrictive underlying mathematical assumptions of the standard measures. As demonstrated on the test data, allowing for a systematic distinction between different dependence and independence combinations of category relations in the data, the proposed measure provides new insights into populational differences between SNP relations in the Alzheimer-relevant gene regions and opens new possibilities for Genome Wide Association Studies (GWAS).

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MS70

Multi-Resolution Dynamic Mode Decomposition and Koopman Theory

We integrate the dynamic mode decomposition (DMD) with a multi-resolution analysis which allows for a decomposition method capable of robustly separating complex systems into a hierarchy of multi-resolution time-scale components. A one-level separation allows for background (low-rank) and foreground (sparse) separation of dynamical data, or robust principal component analysis. The multi-resolution dynamic mode decomposition is capable of characterizing nonlinear dynamical systems in an equation-free manner by recursively decomposing the state of the system into low-rank terms whose temporal coefficients in time are known. It also has a strong connection to Koopman theory which allows for projecting the nonlinear dynamics onto an infinite-dimensional linear operator. DMD modes with temporal frequencies near the origin (zero-modes) are interpreted as background (low-rank) portions of the given dynamics, and the terms with temporal frequencies bounded away from the origin are their sparse counterparts. The multi-resolution dynamic mode decomposition (mrDMD) method is demonstrated on several examples involving multi-scale dynamical data, showing excellent decomposition results, including sifting the El Nino mode from ocean temperature data. It is further applied to decompose a video data set into separate objects moving at different rates against a slowly varying background. These examples show that the decomposition is an effective dynamical systems tool for data-driven discovery.

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MS70

Reduced Order Precursors of Rare Events in Unidirectional Nonlinear Water Waves

Abstract not available.

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MS70

A Transfer Operator Approach to the Prediction of Atmospheric Regime Transition

The existence of persistent midlatitude atmospheric flow regimes with time-scales larger than 510 days and indications of preferred transition paths between them motivates to develop early warning indicators for such regime transitions. While ergodic theory provides a valuable framework for prediction and uncertainty quantification in chaotic or stochastic systems, only recently has a reduction method been proposed to approximate transfer operators governing the evolution of statistics. This method is applied to a hemispheric barotropic model to develop an early warning indicator of the zonal to blocked flow transition in this model. It is shown that the spectrum of the transfer operators can be used to study the slow dynamics of the flow as well as the non-Markovian character of the reduction. The slowest motions are thereby found to have time scales of three to six weeks and to be associated with meta-stable regimes (and their transitions). These regimes can be detected as almost-invariant sets of the transfer operators and are associated regions of low kinetic energy. Furthermore, the reduced operators are used to design an early warning indicator of transition which is statistical in nature, allowing to asses forecast uncertainty. Even though the model is highly simplified, the skill of the early warning indicator is promising, suggesting that the transfer operator approach can be used in parallel to an operational deterministic model for stochastic prediction or to assess forecast uncertainty.

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MS71

The Role of Global Sensitivity Analysis in Interpreting Subsurface Processes under Uncertainty

Global sensitivity analysis (GSA) projects uncertainty of input parameters onto the variance of model responses, leading to improved characterization of complex systems and assisting design of measurement networks. GSA is compatible with model discrimination criteria and allows assessing contributions of model uncertainty to the overall system variability. Examples are presented to showcase the role of GSA in interpreting groundwater flow/transport processes, where quantification of uncertainty associated with model predictions is critical to design management strategies.

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MS71

Estimating Flow Parameters for the Unsaturated Zone Using Data Assimilation

Prediction of soil moisture is an important component in many land surface models. The Ensemble Kalman filter has become a popular method to integrate time series of observations into predictions. Updating hydraulic parameters in the filter is often done using an augmented state approach, as parameters might be not known. We discuss the feasibility of parameter estimation for soils in these settings with a focus on the presence of model errors and compare different filters.

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MS71

An Adaptive Sparse Grid Algorithm for Darcy Problems with Log-normal Permeability

In this talk we propose a modified version of the classical adaptive sparse grid algorithm, that handles non-nested collocation points and an infinite number of input parameters with unbounded support. We then use it to solve the Darcy equation a with lognormal permeability random field that has a Matern covariance function. In case of rough permeability fields, we propose to use the adaptive sparse grid as a control variate to a Monte Carlo estimator.

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MS72

Uncertainty Quantification Python Laboratory (UQ-PyL) A GUI For Parametric Uncertainty Analysis of Large Complex Dynamical Models

This paper describes the newly developed Uncertainty Quantification Python Laboratory (UQ-PyL), a software platform designed to quantify parametric uncertainty of complex dynamical models. UQ-PyL integrates different UQ methods, including experimental design, statistical analysis, sensitivity analysis, surrogate modeling and parameter optimization. It is written in Python with a graphical user interface (GUI) and runs on all common operating systems. In this presentation, we illustrate the different functions of UQ-PyL through some case studies.

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MS72

Advancements in the Uqlab Framework for Uncertainty Quantification

The UQLab software framework is a Matlab-based modular platform that allows users from different fields and without extensive programming background to access and develop state-of-the-art algorithms for uncertainty quantification. Since the public beta testing phase started in July 2015, a number of improvements and new features have been added, making UQLab appealing to many different applied research fields. A general overview of the current features of the framework and selected case studies are presented.

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MS72

PSUADE: A Software Toolkit for Uncertainty Quantification

PSUADE is an software system for analyzing the relationships between the inputs and outputs of general multiphysics simulation models for the purpose of performing uncertainty and sensitivity analyses. In this talk the general capabilities of PSUADE will be highlighted and its design will be discussed. Several applications will also be given to illustrate its capabilities.

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MS73

A Multi-Level Compressed Sensing Petrov Galerkin Method for the Approximation of Parametric PDEs

In this talk, we review the use of compressed sensing and its weighted version in the context of high dimensional parametric and stochastic PDEs. We see that under some rather weak summability and ellipticity assumptions, the polynomial chaos expansion of the solution map shows some compressibility property. We further derive a multilevel scheme to speed up the calculations, leading to a method that has a computational cost in the order of a single PDE solve at the finest level of approximation and still has reliable guarantees.

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MS73

CORSING: Sparse Approximation of PDEs Based on Compressed Sensing

Establishing an analogy between the sampling of a signal and the Petrov-Galerkin discretization of a PDE, the CORSING method can recover the best s-term approximation to the solution with respect to N suitable trial functions, with $s \ll N$, by evaluating the bilinear form associated with the PDE against a randomized choice of $m \ll N$ test functions. This yields an underdetermined $m \times N$ linear system, that is solved by means of sparse optimization techniques.

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MS73

Multilevel Monte-Carlo Hybrids Exploiting Multi-fidelity Modeling and Sparse Polynomial Chaos

In this talk, we present recent experience in developing multilevel Monte Carlo (MLMC) methods that relax the direct tie to a sequence of discretization levels for a particular model form. Of particular interest are (1) extension of MLMC methods to the general multifidelity setting with an ensemble of distinct model forms, and (2) hybridization with polynomial chaos expansion methods based on sparse recovery in order to increase statistical estimator performance within the MLMC framework. Numerical results for multiple discretization levels and multiple model forms will be presented.

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MS73

Posterior Concentration and High Order Quasi Monte Carlo for Bayesian Inverse Problems

We analyze combined Quasi-Monte Carlo quadrature and Finite Element approximations in Bayesian estimation of solutions to countably-parametric operator equations with holomorphic dependence on the parameters considered in [Cl. Schillings and Ch. Schwab: Sparsity in Bayesian Inversion of Parametric Operator Equations. Inverse Problems, **30**, (2014)]. Such problems arise in numerical uncertainty quantification and in Bayesian inversion of operator equations with distributed uncertain inputs, such as uncertain coefficients, uncertain domains or uncertain source terms and boundary data. It implies, in particular, regularity of the parametric solution and of the countably-parametric Bayesian posterior density in SPOD weighted spaces. This, in turn, implies that the Quasi-Monte Carlo quadrature methods in [J. Dick, F.Y. Kuo, Q.T. Le Gia, D. Nuyens, Ch. Schwab, Higher order QMC Galerkin discretization for parametric operator equations, SINUM (2014)] are applicable to these problem classes, with dimension-independent convergence rates. We address the impact of posterior concentration, due to small observation noise covariance on the error bounds, and present numerical results.

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MS74

Model Adaptivity in Bayesian Inverse Problems

Many Bayesian inverse problems involve computationally expensive forward models. When the inference parameters implicitly define the forward model, an additional complexity arises in choosing appropriate discretizations of the model parameters and state; this choice affects both the accuracy of the posterior and the convergence rates of posterior sampling schemes. The inference of uncertain parameters in PDEs is one such example. We explore this problem by developing posterior-focused error estimates and adaptivity criteria that combine adaptive procedures for deterministic inverse problems with Markov chain Monte Carlo sampling.

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MS74

A Multifidelity Stochastic CFD Framework for Robust Simulation with Gappy Data

We develop a general CFD framework based on multifidelity simulations with gappy domains, called gappy simulation. We combine approximation theory, domain decomposition, and patch dynamics together with machine learning techniques, e.g., coKriging, to estimate local boundary of non-overlapped patches. From gaps between individual patches, we observe and analyze uncertainty quantification by two different benchmark problems with general finite difference methods. Finally, we set the foundations for a new class of robust algorithm for stochastic CFD.

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MS74

Tree-Structured Expectation Propagation for Stochastic Multiscale Differential Equations

We develop a hierarchical conditional random field model using tree-structured Expectation Propagation (EP) as a surrogate for multiscale stochastic PDEs. Hidden variables are introduced to capture coarse graining effects and are then integrated out for inference. EP can give predictions on new inputs as well as quantify uncertainties in the output whilst dealing with the local correlations within the cliques. We present applications of the model on stochastic ODEs and PDEs.

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MS74

Multi-Fidelity Simulation of Random Fields by Multi-Variate Gaussian Process Regression

In this talk outline a general procedure that employs recursive Bayesian network techniques and multiple information sources with different levels of fidelity to predict the statistical properties of random fluid systems. In particular, we address the problem of how to construct optimal predictors for quantities of interest such as the temperature field in stochastic Rayleigh-Benard convection. The effectiveness of the new algorithms is demonstrated in numerical examples involving prototype stochastic PDEs.

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MS75

Subset Simulation: Strategies to Enhance the Performance of the Method

Subset Simulation is an adaptive Monte Carlo method that is efficient for estimating small probabilities in high dimensional problems. We present strategies to improve the MCMC sampling in Subset Simulation. This includes a simple yet efficient proposal distribution, as well as an algorithm to adaptively learn the spread of the proposal distribution. Furthermore, we investigate the influence of dependent MCMC seeds on the variability of the computed probability.

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MS75

Markov Chain Monte Carlo for Rare Event Reliability Analysis with Nonlinear Finite Elements

Many structural design problems are highly nonlinear and are often required to have very small probabilities of failure. Nonlinear finite element analysis can be combined with Subset Simulation for efficient calculation of rare event probabilities in physical models with spatially autocorrelated material parameters. Reliability analysis for nonlinear problems provides distinct challenges in addition to those encountered in linear problems. These challenges are discussed with reference to a practical test case, a footing on elastoplastic soil.

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MS75

Multilevel Monte Carlo Methods for Computing Failure Probability of Porous Media Flow Systems

We study improvements of Monte Carlo (MC) methods for point evaluation of the cumulative distribution function of quantities from porous media two-phase flow models with uncertain permeability. We consider indicators for the capacity of CO_2 storage systems, e.g. sweep efficiency. We quantify the computational gains using recent MC improvements: selective refinement and multilevel MC. Compared to MC, the computational effort can be reduced one order of magnitude for typical error tolerances.

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MS75

Bayesian Updating of Rare Events: The BUS Approach

We present an efficient framework to performing Bayesian updating of rare event probabilities, termed BUS. It is based on a reinterpretation of the classical rejection-sampling approach to Bayesian analysis, combined with established methods for estimating probabilities of rare events. These methods include the First-Order Reliability Method (FORM), importance sampling methods as well as subset simulation. We showcase the applicability of the BUS approach with numerical examples involving stochastic PDEs in one and two-dimensional physical space.

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MS76

Numerical Integration of Piecewise Smooth Systems

Many applications involve functions that are piecewise smooth with kinks or jumps at the interfaces. Provided the functions are given by evaluation procedures these discontinuities can be located quite accurately and the numerical purpose, be it high dimensional quadrature or more general the numerical integration of dynamical systems can sometimes be achieved without a significant loss of accuracy or efficiency compared to the smooth case. We discuss suitable scenarios for this to be the case.

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MS76

Gpu Acceleration of the Stochastic Grid Bundling Method for Early-Exercise Options

Pricing early-exercise options under multi-dimensional stochastic processes is a major challenge in the financial sector. In this work, a parallel GPU version of the Monte Carlo based Stochastic Grid Bundling Method (SGBM) [Shashi Jain and Cornelis W. Oosterlee. The Stochastic Grid Bundling Method: Efficient pricing of Bermudan options and their Greeks. Applied Mathematics and Computation, 269: 412-431, 2015] for pricing multi-dimensional Bermudan options is presented. To extend the method's applicability, the problem dimensionality will be increased drastically. This makes SGBM very expensive in terms of computational cost. A parallelization strategy of the method is developed by employing GPGPU paradigm.

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MS76

On Tensor Product Approximation of Analytic Functions

We discuss tensor products of certain univariate approximation schemes for multivariate functions that are analytic in certain polydiscs. In the finite-variate setting we prove exponential error bounds, while for the infinite-variate case we prove algebraic and sub-exponential bounds.

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MS76

Numerical Solution of Elliptic Diffusion Problems on Random Domains

In this talk, we provide regularity results for the solution to elliptic diffusion problems on random domains. In particular, based on the decay of the Karhunen-Loeve expansion of the domain perturbation field, we establish rates of decay of the solutions derivatives. This anisotropy can be exploited in a sparse quadrature to compute quantities of interest of the solution. In combination with parametric finite elements, we end up with a non-intrusive and efficient method.

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MS77

Uncertainty Quantification of a Tsunami Model with Uncertain Bathymetry Using Statistical Emulation

VOLNA, a nonlinear shallow water equations solver, produces high resolution simulations of earthquake-generated tsunamis. However, the uncertainties in the bathymetry (seafloor elevation) have an impact on tsunami waves. We quantify the bathymetry as random fields which are parametrised as inputs of VOLNA. Because of the high-dimensionality of these inputs, we propose a joint framework of statistical emulation with dimension reduction procedure for uncertainty quantification to obtain reliable probabilistic assessment of tsunami hazard.

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MS77

A Measure-Theoretic Approach to Parameter Estimation

In this talk, we will discuss the application of a new measure-theoretic approach to parameter estimation. The measure theoretic approach is based on computing the probability of events in parameter space, given the probability of measurable events in data space. We will describe the application of this methodology to two complex problems: the estimation of parameter fields within a coastal ocean model, and the estimation of transport parameters in a groundwater contamination model.

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MS77

An Overview of Uncertainty Quantification in Geophysical Hazard Analyses

Simulation based studies (and often surrogates to make UQ tractable) are essential in geophysical hazard analyses given the rare nature of devastating hazards and limited observational data. I will give an overview of approaches, methodologies, and challenges that arise in quantifying uncertainty in simulation-aided geophysical hazard assessment.

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MS77

Uncertainty Quantification About Dynamic Flow, Frequency, and Initiation of Pyroclastic Flows

Decade-long observations of initiation angles for Pyroclastic Flows at the Soufriere Hills Volcano in Montserrat show little departure from a uniform distribution on the circle, but short-term studies tell a different story— angles are similar for consecutive groups of smaller eruptions between major dome-collapse events. In the hope of making more accurate short-term hazard assessment and forecasts, we build and fit dynamic models of flow, frequency, and initiation angles for Pyroclastic Flows.

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MS78

Title Not Available

Abstract not available.

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MS78

Uncertainty Quantification in 4D Seismic

In seismic imaging, multiple large data sets are often collected to monitor a producing reservoir. These data are then analyzed to image changes in the subsurface. Because of the inherent non-uniqueness of the seismic inverse problem, it is difficult to determine which changes are real. This presentation will detail how we can use the multiple data sets available in this case to efficiently compute a confidence map and relate it to the inherent uncertainties.

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MS78

A Randomized Misfit Approach for Data Reduction in Large-Scale Inverse Problems

We present a randomized misfit approach (RMA) for efficient data reduction in large-scale inverse problems. The method is a random transformation approach that generates reduced data by randomly combining the original ones. The main idea is to first randomize the misfit and then use the sample average approximation to solve the resulting stochastic optimization problem. At the heart of our approach is the blending of the stochastic programming and the random projection theories, which brings together the advances from both sides. One of the main results of the paper is the interplay between the Johnson-Lindenstrauss lemma and large deviation theory. A tight connection between the Morozov discrepancy principle and the Johnson-Lindenstrauss lemma is presented. Various numerical results to motivate and to verify our theoretical findings are presented for inverse problems governed by elliptic partial differential equations in one, two, and three dimensions.

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MS78

Sub-sampled Newton Methods and Modern Big Data Problems

Many data analysis applications require the solution of optimization problems involving a sum of large number of functions. We consider the problem of minimizing a sum

of n functions over a convex constraint set. Algorithms that carefully sub-sample to reduce n can improve the computational efficiency, while maintaining the original convergence properties. For second order methods, we give quantitative convergence results for variants of Newtons methods where the Hessian or the gradient is uniformly sub-sampled.

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MS79

Improved Dynamic Mode Decomposition Algorithms for Noisy Data

The dynamic mode decomposition (DMD) algorithm gives a means to extract dynamical information and models directly from data. The practical utility of DMD, however, can be hindered by a sensitivity to noisy data. We show that DMD is biased to measurement noise, and discuss a number of noise-robust modifications to the algorithm that remove this bias. We further demonstrate how these approaches can be extended to improve related data-driven modeling algorithms.

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MS79

Temporal Compressive Sensing of Strain Histories of Compliant Wings for Classification of Aerodynamic Regimes

Mechanosensory flight control in insects is moderated by *campaniform sensilla* or strain sensors along wings that collect information from aerodynamic environment. We speculate that sparse strain measurements that encode aerodynamic loading are sufficient to detect the presence of fluid instabilities and robustly differentiate aerodynamic disturbances. To confirm this, strain data is obtained from a numerical fluid-structure model of a compliant flapping hawkmoth wing. A comparison of dominant features of spatial and temporal strain signatures reveals that temporal strain histories are crucial for distinguishing different aerodynamic environments. Next, regime identification is recast as a classification problem of fitting a temporal strain history into a rich matrix library of frequency features obtained from different aerodynamical regimes. By integrating additive sensor noise, we demonstrate robust classification of new strain histories into the library using ℓ_1 minimization to promote sparsity in the discriminating coefficients. Finally we examine classification accuracy for frequency windows that best separate the signals by integrating compressive sensing and bandlimited sampling of strain frequency features.

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MS79

Uncertainty Analysis - An Operator Theoretic Approach

Abstract not available.

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MS79

Discovering Dynamics from Measurements, Inputs, and Delays

Abstract not available.

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MS80

A Constructive Method for Generating Near Minimax Distance Designs

We propose a new class of space-filling designs called rotated sphere packing designs. The approach starts from the asymptotically optimal positioning of identical balls that covers the unit cube. Properly scaled, rotated, translated and extracted, such designs are near optimal in minimax distance criterion, low in discrepancy, good in projective uniformity and thus useful in both prediction and numerical integration purposes. The proposed designs can be constructed for any given numbers of dimensions and points.

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MS80

Smoothed Brownian Kriging Models for Computer Simulations

Gaussian processes have become a common framework for modeling deterministic computer simulations and producing predictions of the response surface. This talk discusses why the ubiquitous radial covaraince assumption is limiting in terms of the long range behavior of the response surface. To avoid this problem, this talk proposes a new, non-radial covariance function . Twelve examples indicate that the use of this covariance can result in better predictions on realistic problems.

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MS80

A Submodular Criterion for Space-Filling Design

We propose a new criterion for space-filling design in computer experiments, based on the notion of covering measure, indexed by a nonnegative scalar q. It is submodular and is related to the minimax-distance criterion for large q. Its submodularity implies that a simple greedy optimization yields a design sequence that satisfies guaranteed efficiency bounds. Various examples compare performance achieved in terms of minimax optimality for moderate input dimension d to existing space filling methods.

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MS80

An Iterative Procedure for Large-scale Computer Experiments

In this paper we propose an iterative procedure to fit large-scale computer experiments. This procedure avoids the computation of matrix inverse, and then yields a class of computational cheaper and more stable emulators. In addition, with the interpolation property in each iteration, our procedure can improve a cheap linear emulator in one or several iterations. Numerical examples are presented to illustrate our method. (joint work with Peter Z G Qian)

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MS81

A Hybrid Ensemble Transform Filter for High Dimensional Dynamical Systems

Data assimilation is the task to combine evolution models and observational data in order to produce reliable predictions. In this talk, we focus on ensemble-based recursive data assimilation problems. Our main contribution is a hybrid filter that allows one to adaptively bridge between ensemble Kalman and particle filters. While ensemble Kalman filters are robust and applicable to high dimensional problems, particle filters are asymptotically consistent in the large ensemble size limit. We demonstrate numerically that our hybrid approach can improve the performance of both Kalman and particle filters at moderate ensemble sizes. We also show how to implement the concept of localisation into a hybrid filter, which is key to their applicability to high dimensional problems.

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MS81

Bayesian Smoothing and Learning for Multiscale Ocean Flows

We illustrate a Bayesian inference methodology that allows the joint inference of the state, equations, geometry, boundary conditions and initial conditions of dynamical models. The learning methodology combines the adaptive reduced-order Dynamically-Orthogonal (DO) stochastic partial differential equations with Gaussian Mixture Models (GMMs). To learn backward in time, we utilize a novel Bayesian smoother for high-dimensional continuous stochastic fields governed by general nonlinear dynamics, the GMM-DO smoother. Examples are provided for time-dependent fluid and ocean flows, including Strait flows with jets and eddies, and multiscale bottom gravity currents. This is joint work with our MSEAS group at MIT.

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MS81

Stability of Ensemble Kalman Filters

The ensemble Kalman filters are data assimilation methods for high dimensional, nonlinear dynamical models. Despite their widespread usage, very little is known about their long-time dynamical behavior. In this talk, we discuss the criterions that guarantee the filter ensemble to be time uniformly bounded and geometrically ergodic. Contradiction of these criterions may lead to catastrophic filter divergence through a concrete example. Finally, we show that a simple adaptive covariance inflation scheme can guarantee filter stability.

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MS81

Uncertainty Propagation for Bilinear Pdes: the Minimax Approach

Abstract not available.

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MS82

Low-rank Approximation Method for the Solution of Dynamical Systems with Uncertain Parameters

Low-rank approximation methods are receiving a growing attention for solving multi-parametric problems, especially arising in the context of uncertainty quantification. Here, we propose a low-rank approximation method, with a subspace point of view, for the solution of non linear dynamical systems with uncertain parameters. The method relies on the construction of an increasing sequence of time dependent reduced spaces in which the full model is projected to derive the reduced dynamical system. The basis of the reduced spaces is selected in a greedy fashion among samples of the solution trajectories using efficient a posteriori error estimates.

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MS82

Alternating Iteration for Low-Rank Solution of the Inverse Stochastic Stokes Equation

High-dimensional partial differential equations arise naturally if spatial coordinates are extended by time and auxiliary variables. The latter may account for uncertain inputs or design parameters. After discretization, the number of degrees of freedom grows exponentially with the number of parameters. To reduce the complexity, we can employ the separation of variables and approximate large vectors and matrices by a polylinear combination of factors, each of whose depends only on one variable. One of the most powerful combinations are Tensor Train and Hierarchical Tucker decompositions. A workhorse method to compute the factors directly is the Alternating Least Squares iteration and its extensions. However, it was too difficult to treat matrices of a saddle point structure via existing alternating schemes. Such matrices appear in an optimal control problem, where a convex optimization, constrained by a high-dimensional PDE, is solved via Lagrangian approach. In this talk, we show how to preserve the saddle-point structure of the linear system during the alternating iteration and solve it efficiently. We demonstrate numerical examples of the inverse Stokes-Brinkman and Navier-Stokes problems.

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MS82

On the Convergence of Alternating Least Squares Optimisation in Tensor Format Representations

The approximation of tensors is important for the efficient numerical treatment of high dimensional problems, but it remains an extremely challenging task. One of the most popular approach to tensor approximation is the alternating least squares method. In our study, the convergence of the alternating least squares algorithm is considered. The analysis is done for arbitrary tensor format representations and based on the multiliearity of the tensor format. In tensor format representation techniques, tensors are approximated by multilinear combinations of objects lower dimensionality. The resulting reduction of dimensionality not only reduces the amount of required storage but also the computational effort.

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MS82

Parallel Low Rank Tensor Arithmetics for Extreme Scale UQ

Solutions of high-dimensional problems can be approximated as tensors in the Hierarchical Tucker Format, if the dependency on the parameters fulfills a low rank property. Our goal is to perform arithmetics for tensors in the Hierarchical Format, where a tensor is supposed to be distributed among several compute nodes, as it may arise from a parallel approximation algorithm. This allows for parallelization of the arithmetic operations, which are e.g. the truncation of a tensor to a certain rank or the application of an operator to a tensor. When the operator as well as the right-hand side of a PDE are given in the Hierarchical Format, one can compute the residual of a solution directly in the Hierarchical Format.

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MS83

A Partial Domain Inversion Approach for Large-scale Baysian Inverse Problems in High Dimensional Parameter Spaces

While Bayesian inference is a systematic approach to account for uncertainties, it is often prohibitively expensive for inverse problems with large-scale forward equation in high dimensional parameter space. We shall develop a *partial domain inversion strategy* to only invert for distributed parameters that are well-informed by the data. This is an efficient data-driven reduction method for both forward equation and parameter space. This approach induces several advantages over existing methods. First, depending on the size of truncated domain, solving the truncated forward equation could be much less computationally demanding. Consequently, the adjoint (and possibly incremental forward and adjoint equations if Newton-like method is used is much less computationally intensive. Second, since the parameter to be inverted for is now restricted, the curse of dimensionality encountered when exploring the parameter spaces (to compute statistics of the posterior density, for example) is mitigated. We present both deterministic inversion and statistical inversion with Monte Carlo approaches.

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MS83

Higher-Order Quasi-Monte Carlo Integration in Bayesian Inversion

An important problem in uncertainty quantification, in particular when considering the Bayesian approach to inverse problems, is the approximation of high-dimensional integrals. We consider novel quasi-Monte Carlo (QMC) methods for tackling such problems, which aim to outperform existing methods by achieving higher orders of convergence. The methods presented in this talk are based on *interlaced polynomial lattice rules* and allow, for certain integrands, a convergence behavior of the quadrature error of $\mathcal{O}(N^{-\alpha})$ with $\alpha \geq 2$ [Dick, Kuo, Le Gia, Nuyens, Schwab, *Higher order QMC Petrov-Galerkin discretization for affine parametric operator equations with random field inputs.* SIAM J. Numerical Analysis **52**(6) (2014).], [Gantner, Schwab, *Computational Higher Order Quasi-Monte Carlo Integration* (2014).] We mention the assumptions on the forward model required to obtain these better rates, and give some results of both forward and Bayesian inverse UQ of certain partial differential equation (PDE) models [Dick, Le Gia, Schwab, *Higher-order quasi-Monte Carlo integration for holomorphic, parametric operator equations.* Tech. Rep. 2014-23, Seminar for Applied Mathematics, ETH Zurich (2014).]

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MS83

Hierarchical Bayesian Level Set Inversion

The level set approach has proven widely successful in the study of inverse problems, since its systematic development in the 1990s. Recently it has been employed in the context of Bayesian inversion, allowing for the quantification of uncertainty within reconstruction methods. However the Bayesian approach is very sensitive to the length and amplitude scales encoded in the prior probabilistic model. This paper demonstrates how the scale-sensitivity can be circumvented by means of a hierarchical approach, using a single scalar parameter. Together with careful consideration of the development of algorithms which encode probability measure equivalences as the hierarchical parameter is varied, this leads to well-defined Gibbs based MCMC methods found by alternating Metropolis-Hastings updates of the level set function and the hierarchical parameter. These methods are demonstrated to outperform non-hierarchical Bayesian level set methods.

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MS83

Discrete Monge-Kantorovich Approach for Sampling Bayesian Posteriors

Sampling techniques are important for large-scale high dimensional Bayesian inferences. However, general-purpose technique such as Markov chain Monte Carlo is intractable. We present an ensemble transform algorithm that is rooted from a discretization of the Monge-Kantarovich transport problem. The method transforms the prior ensemble to posterior one via a sparse optimization. We develop methods to accelerate the computation of the transformation. Numerical results for large-scale Bayesian inverse problems governed by PDEs will be presented.

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MS84

Uncertainty Quantification for Modeling Night-Time Ventilation in Stanford's Y2E2 Building

A variety of models, ranging from box models that solve for the volume-averaged air and thermal mass temperatures to detailed CFD models, can be used to predict natural ventilation performance. The simplifications and assumptions introduced in these models can result in significant uncertainty in the results. This study investigates the predictive capability of a box model and a CFD model for night-flush ventilation in the Y2E2 building, and compares the results with available temperature measurements.

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MS84

Epistemic Uncertainty Quantification of the Sec-

ond Moment Closure Turbulence Modeling Framework

Predictive turbulence calculations require that the uncertainty in various constituent closures is quantified. We propose that uncertainty quantification must commence at the Reynolds stress closure level. The Reynolds stress tensor provides an insufficient basis to describe the internal structure of a turbulent field, expressly its dimensionality. It is demonstrated that this leads to an inherent degree of uncertainty in classical models for turbulent flows. We quantify the propagation of this epistemic uncertainty for different regimes of mean flow. It is exhibited that the magnitude of this uncertainty is dependent not just upon the dimensionality of the turbulent field, but to a greater degree upon the nature of the mean flow. Finally, we analyze the qualitative and quantitative effects of the non-linear component of pressure on this systemic uncertainty.

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MS84

Reducing Epistemic Uncertainty of Fluid-Structure Instabilities

Aeroelastic problems contain a computationally intensive aerodynamic part, and a relatively cheap structure part. Two reduced-order modeling strategies based on system identification, namely AutoRegression with eXogenous inputs (ARX), and a Linear Parameter Varying (LPV) model, are employed to build a reduced aerodynamic solver. This model is then coupled with the full-order structural solver in order to update the aeroelastic solution. Propogating uncertainty on structural parameters becomes cheap, and Bayesian idenification of stability boundaries is performed.

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MS84

Quantifying and Reducing Model-Form Uncertainties in Reynolds Averaged Navier-Stokes Simulations: An Open-Box, Physics-Based, Bayesian Approach

RANS models are the workhorse tools for turbulent flow simulations in engineering design an optimization. For many flows the turbulence models are by far the most important source of uncertainty in RANS simulations. In this work we develop an open-box, physics-informed Bayesian framework for quantifying model-form uncertainties in RANS simulations. An iterative ensemble Kalman method is used to assimilate the prior knowledge and observation data. The framework is a major improvement over existing black-box methods.

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MS85

Calibration of Velocity Moments from Experimental and Les Simulation Data

Reynolds Averaged Navier Stokes (RANS) are the workhorse of turbulence simulations, but the parameters vary from problem to problem and require setting from external sources. A key parameter is turbulent kinetic energy, TKE, a second moment of the turbulent velocity statistics. Here we study verification, validation and uncertainty quantification for this quantity, while addressing three very distinct flows, related to inertial confinement fusion, solar energy collectors and meteorological wind currents.

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MS85

Uncertainty Quantification for the Simulation of Bubbly Flows

The direct numerical simulation method for bubbly flows based on the front tracking technique has been used for the simulations of the propagation of linear and shock waves. The uncertatinties in the quantity of interests (QoI) such as the peak pressures and the collapse time depending on the initial conditions are studied. The goal is to reduce the uncertainties in the QoI based on the collection of initial conditions and perform efficient simulations to predict the collapse of cavitation bubbles.

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MS85

Model Validation for Porous Media Flows

We present a new Bayesian framework for the validation of subsurface flow models. We use a compositional model to simulate CO2 injection in a core, and compare simulated to observed saturations. We first present computational experiments involving a synthetic permeability field. They show that the framework captures almost all the information about the heterogeneity of the permeability field of the core. We then apply the framework to real cores, using data measured in the laboratory.

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MS85

Recent Developments in High-Order Stochastic Finite Volume Method for the Uncertainty Quantifi-

cation in Cfd Problems

We develop the Stochastic Finite Volume (SFV) method for uncertainty quantification based on the parametrization of the probability space and the numerical solution of an equivalent high-dimensional deterministic problem. To this end, standard numerical approaches like finite volume or discontinuous Galerkin can be used to approximate the numerical solution of the parametrized equations, thus allowing for a natural way to achieve a high order of accuracy and an easy calculation of the statistical quantities of interest at the postprocessing stage. We derive the error estimates for the mean and variance resulting from the SFVM and show that the convergence rates of the statistical quantities are equivalent to the convergence rates of the deterministic solution. We have also proposed an anisotropic discretization of the stochastic space which increases the computational efficiency of the SFV method. The resolution capabilities of the SFV method are compared to Multi-Level Monte carlo method. We finally generalize the SFVM approach and apply the DG discretization on the unstructured triangular (in 2D) or tetrahedral (in 3D) grids in the physical space. We demonstrate the efficiency the implemented method on various numerical tests.

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MS86

Machine Learning Assisted Sampling Algorithm for Inverse Uncertainty Quantification

An efficient Bayesian sampling algorithm for calibration of subsurface reservoirs is proposed. It builds on the nested sampling (NS) algorithm [Skilling, 2006] for obtaining samples from the posterior distribution of the model parameters. The main idea of nested sampling is to reformulate the posterior sampling problem into a sequence of likelihood constraint prior sampling sub-problems with increasing complexity. Initially, the likelihood constraint is set to a low value and the prior constrained sampling is relatively easy to perform. At later stages of the NS algorithm, the likelihood constraint is set to higher value and the constrained sampling is much harder to perform. In the current work, we combine nested sampling with a machine learning based classification algorithm to accelerate the constrained sampling step. Further, we apply an annealing technique for problems with very localized regions of attraction. This results in two-way splitting of the posterior sampling problem both in the likelihood value (using nested sampling) and in the likelihood surface complexity (using an annealing schedule). Numerical evaluation is presented for calibration and prior model section of nonlinear problems representing the two-phase flow in subsurface reservoirs.

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MS86

Application of Multilevel Concepts for Uncertainty Quantification in Reservoir Simulation

Uncertainty quantification is an important task in reservoir simulation. The main idea of uncertainty quantification is to compute the distribution of a quantity of interest, for example, field oil production rate. That uncertainty, then feeds into the decision making process. A statistically valid way of quantifying the uncertainty is a Markov Chain Monte Carlo (MCMC) method, such as Metropolis-Hastings (MH). MH can be prohibitively expensive when the function evaluates take a long time as is the case in reservoir simulation. There are different techniques accelerate the convergence for MH, e.g., Hamiltonian Monte Carlo (HMC) and Multilevel Markov Chain Monte Carlo (MLMCMC). MLMCMC is based on using the multilevel concept to accelerate the MH convergence. In this paper, we show how to use the multilevel concept in different scenarios for quantifying uncertainty in reservoir simulation. We discuss the performance of the new techniques based on the result for real field in the central Gulf of Mexico.

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MS86

Accelerating Uncertainty Quantification with Proxy and Error Models

To reduce the computational cost of stochastic approaches in hydrogeology, one often resorts to approximate flow solvers (or proxy). Error models are then necessary to correct proxy responses for inference purposes. We propose a new methodology based on machine learning tools and we employ an iterative scheme to construct an error model that allows us to improve and evaluate its performance. The results are illustrated with a nested sampling example.

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MS86

Bayesian Hierarchical Model in Spatial Inverse Problems

We consider a Bayesian approach to nonlinear inverse problems in which the unknown quantity is a random spatial field. The Bayesian approach contains a natural mechanism for regularization in the form of prior information, can incorporate information from heterogeneous sources and provide a quantitative assessment of uncertainty in the inverse solution. The Bayesian setting casts the inverse solution as a posterior probability distribution over the model parameters. Karhunen- Loeve expansion is used for dimension reduction of the random spatial field. Furthermore, we use a hierarchical Bayes model to inject multiscale data in the modeling framework. In this Bayesian framework, we show that this inverse problem is well-posed by proving that the posterior measure is Lipschitz continuous with respect to the data in total variation norm. Computational challenges in this construction arise from the need for repeated evaluations of the forward model (e.g. in the context of MCMC) and are compounded by high dimensionality of the posterior. We develop two-stage reversible jump MCMC which has the ability to screen the bad proposals in the first inexpensive stage. Numerical results are presented by analyzing simulated as well as real data from hydrocarbon reservoir.

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MS87

Multi-Index Stochastic Collocation

We present the novel Multi-Index Stochastic Collocation method (MISC) for computing statistics of the solution of a PDE with random data. MISC is a combination technique using mixed differences of spatial approximations and quadratures over random data. We provide (i) an optimal selection of the most effective mixed differences to include in MISC, (ii) a complexity analysis and (iii) a numerical study showing its effectiveness, comparing it with other related methods available in the literature.

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MS87

Best S-Term Polynomial Approximations Via Compressed Sensing for High-Dimensional Parameterized Pdes

In this talk we present a weighted ℓ_1 minimization, with a novel choice of weights, and a new iterative hard thresholding method that both exploit the structure of the best s-term polynomial approximation of parameterized PDEs. In addition, we extend the compressed sensing (CS) approach to multidimensional Hilbert-valued signals. Finally, the recovery of our proposed methods is established through an improved estimate of restricted isometry property (RIP), whose proof will also be discussed. Numerical tests will be provided for supporting the theory and demonstrating the efficiency of our new CS methods compared to those in the literature.

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MS87

Domain Uncertainty for Navier Stokes Equations

We analyze sparsity and regularity of viscous, incompressible flow under uncertainty of the domain of definition. Various versions of domain variation are considered, and the continuous dependence as well as regularity of flow field with respect to variations in the domain are investigated. Sparsity results of the flow field with respect to a countable family of parameters for the domain are established.

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MS87

Gradient-Enhanced Stochastic Collocation Approximations for Uncertainty Quantification

The talk is concerned with stochastic collocation methods with gradient informations, namely, we consider the case where both the function values and derivative informations are avaliable . Particular attention will be given to discrete least-squares and the compressive sampling methods. Stability results of these approaches will be presented.

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MS88

Sensitivity Analysis Methods for Uncertainty Budgeting in System Design

This talk presents a new approach to defining and managing budgets on the acceptable levels of uncertainty in design quantities of interest. Examples of budgets are the allowable risk in not meeting a critical design constraint and the allowable deviation in a system performance metric. A sensitivity-based method analyzes the effects of design decisions on satisfying those budgets, and a multi-objective optimization formulation permits the designer to explore the tradespace of uncertainty reduction activities while also accounting for a cost budget.

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MS88

A Full-Space Approach to Stochastic Optimization with Simulation Constraints

Full-space methods are an attractive alternative to reduced-space approaches when dealing with nonlinear or rank-deficient simulation constraints in engineering applications. We analyze the theoretical and computational challenges that arise when the simulation constraints include random inputs. For problems constrained by PDEs we discuss several discretization strategies, and present scalable solvers for optimality systems arising in a composite-step sequential quadratic programming scheme. Numerical examples include risk-averse control of thermal fluids.

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MS88

Uncertainty Quantification for Subsurface Flow Problems

The Ensemble Kalman filter (EnKF) has had enormous impact on the applied sciences since its introduction in the 1990s by Evensen and coworkers. In this talk, we will discuss an analysis of the EnKF based on the continuous time scaling limits, which allows to study the properties of the EnKF for fixed ensemble size. The theoretical considerations give useful insights into properties of the method and provide tools for a systematic development and improvement. Results from realistic petroleum engineering problems with real datasets supporting the theoretical findings will be presented.

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MS88

Risk Averse Optimization for Engineering Applications

Engineering applications often require solutions to multiple optimization problems including inversion, control, and design, in addition to addressing a variety of uncertainties. We demonstrate a strategy that couples uncertainties between inversion and control under uncertainty using risk measures. We demonstrate both risk neutral and CVaR in the context of finding a robust control strategy for the management of atmospheric trace gases.

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MS89

Integrating Reduced-order Models in Bayesian Inference via Error Surrogates

Sampling methods (e.g., MCMC) for statistical inversion can require hundreds of ‘forward solves’ with a computational model. For tractability, high-fidelity models are often replaced with inexpensive surrogates, e.g., reduced-order models (ROMs). However, the epistemic uncertainty introduced by such surrogates is commonly ignored, which leads to errors into the posterior distribution. In this work, we show that employing reduced-order model error surrogates (ROMES) allows ROMs to be rigorously employed for rapid yet rigorous statistical inversion.

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MS89

EIM/GEIM and PBDW Approaches with Noisy Informations

The empirical interpolation method (EIM) and its generalization (GEIM) together with the parametrized-background data-weak (PBDW) approach to variational data assimilation allow to reconstruct states from data in cases where one has some information on the process under consideration. This information is stated through a manifold of the states we are interested in. This manifold can be e.g. the set of all solutions to some parameter dependent PDE. Data are generally noisy and the reconstruction has to take this fact into account. In this talk we are interested in the situation where we want to place optimally the different devices for data acquisition, those possibly i) having a different price, ii) related to a different precision in the measurement and iii) measuring different quantities. The challenge is then, within a given budget, to choose and place the devices so that the knowledge of the state will be the most accurate.

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MS89

Model and Error Reduction for Inverse UQ Problems Governed by Unsteady Nonlinear Pdes

We propose a new Reduced Basis Ensenble Kalman Filter (RB-EKF) for the efficient solution of inverse UQ problems governed by unsteady nonlinear PDEs. Exploiting a Bayesian framework, we combine the RB method for the efficient approximation of the forward problem, an ensemble Kalman filter, and suitable reduced error models to keep under control the propagation of reduction errors. We apply the resulting RB-EKF for identifying both state and parameters/parametric fields in some examples of interest.

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MS89

Goal-oriented Error Estimation

We consider a quantity of interest (QoI), as a functional of the solution of a large system of equations, whose numerical solution is computationally costly. Metamodelling techniques yield a surrogate QoI, which is faster to compute, but can deviate from the original QoI. We apply deterministic (dual-based) and probabilistic methods to derive an error bound between these two quantities of interest. This explicitly computable bound make scarce assumptions about the QoI and the metamodelling technique.

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MS90

Adaptive Simulation for Large Deviations Conditioning

Abstract not available.

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MS90

Rare Event and Subset Simulation for Discontinuous Random Variables

Subset Simulation (SS) aims at estimating extreme probabilities of the form P $[f(\mathbf{U}) > q]$ when f is the real-valued output of a computationally expensive code and $\mathbf{U}$ is a random vector. Discontinuities in the cumulative distribution function of $f(\mathbf{U})$ can make the usual SS estimator not consistent. We present a new consistent version that can be applied without any hypothesis on the discontinuities and that has the same properties as the usual estimator in absence of discontinuity.

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MS90

A Surrogate Accelerated Multicanonical Monte Carlo Method for Uncertainty Quantification

In this work we consider a class of uncertainty quantification problems where the system performance or reliability is characterized by a scalar parameter y. The performance parameter y is random due to the presence of various sources of uncertainty in the system, and our goal is to estimate the probability density function of y. We propose to use the multicanonical Monte Carlo (MMC) method, a special type of adaptive importance sampling algorithm, to compute the PDF of interest. Moreover, we develop an adaptive algorithm to construct local Gaussian process surrogates to further accelerate the MMC iterations. With numerical examples we demonstrate that the proposed method can achieve several orders of magnitudes of speedup over the standard Monte Carlo method.

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MS90

Uniformly Efficient Simulation for the Supremum of Gaussian Random Fields

In this talk, we consider rare-event simulation of the tail probabilities of Gaussian random fields. In particular, we design importance sampling estimators that are uniformly efficient for a family of Gaussian random fields with different mean and variance functions.

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MS91

Openturns for Uncertainty Quantification

OpenTURNS is a scientific C++ library which aims at modeling the uncertainty of inputs of a deterministic simulation and propagating the uncertainties through the model. This library is developed with the open source

LGPL license by four partners: EDF, Airbus Group, Phimeca Engineering and IMACS. Also provided as a Python module, it gathers a growing community of users from various industries.

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MS91

Uranie: the Uncertainty and Optimization Platform

URANIE developed by CEA is a framework to deal with uncertainty and sensitivity analysis, 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 offers several useful functionalities as advanced visualization, powerful data storage and access in several format (ASCII, binary, SQL) and a C++ interpreter.

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MS91

'Mystic': Highly-constrained Non-convex Optimization and Uncertainty Quantification

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 prevalence of parallel computing has stimulated a shift from reduced-dimensional models toward more brute-force methods for solving high-dimensional nonlinear optimization problems. The 'mystic' software enables the solving of difficult UQ problems as embarrassingly parallel non-convex optimizations; and with the OUQ algorithm, can provide validation and certification of standard UQ approaches.

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MS91

Promethee Environment for Computer Code Inversion

The Promethee project aims at spreading design of computer experiments in common engineering practice for many fields of applications. This full stack implementation embeds both distributed computing service, input/output coupling with the targeted computer code and a graphical user interface including the design algorithm. The case study focuses on the Stepwise Uncertainty Reduction algorithm for determination of safety limit in neutronics criticality assessment.

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MS92

Robust Gaussian Stochastic Process Emulation

We consider parameters estimation problems in Gaussian Stochastic Processes (GaSP), which are widely used in computer model emulation. We obtain theoretical results for estimating parameters in a robust way through posterior modes. These results are applicable to many correlation functions, e.g power exponential, Matern, rational quadratic and spherical correlation, along with general designs. Numerical results are studied to demonstrate our better performance than some other methods and R packages.

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MS92

Bayesian Inference of Manning's N Coefficient of a Storm Surge Model: An Ensemble Kalman Filter Vs. a Polynomial Chaos-Mcmc

Bayesian inversion is commonly used to quantify and reduce the uncertainties in coastal ocean models, especially in the framework of parameters estimation. The posterior of the parameters to be estimated is then computed conditioned on available data, either directly using a MCMC method, or by sequentially processing the data following a data assimilation method. The latter approach is heavily exploited in large dimensional state estimation problems and has the advantage to accommodate a large number of parameters without, assumingly, increase in computational cost. However, only approximate posteriors may be obtained by this approach due to the restricted Gaussian prior and noise assumptions that are generally imposed. This contribution aims at evaluating the effectiveness of using an ensemble Kalman-based assimilation method for parameters estimation of a realistic coastal model against an adaptive MCMC Polynomial Chaos (PC)-based approach. We focus on quantifying the uncertainties of the ADCIRC community model w.r.t. the Manning coefficient. We test both constant and variable Manning coefficients. Using realistic OSSEs, we apply an ensemble Kalman filter and the MCMC method based on a surrogate of ADCIRC constructed by a non-intrusive PC expansion, and compare both approaches under identical scenarios. We further study the sensitivity of the estimated posteriors with respect to the inversion method parameters, including ensemble size, inflation factor, and PC order.

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MS92

Adjoint Based Methods for Numerical Error Estimation and Surrogate Construction For Uq and Inverse Problems

In this talk, we will summarize recent work on using adjoint based numerical error estimation of PDE solvers to inform surrogate construction and use in uncertainty quantification. While, it is common to assume that such error is small and does not affect UQ procedures it is often the case that for complex problems and large ensembles (especially for extreme values of parameters) some members of the ensemble can have very large numerical errors. We will show that systematic use of well established numerical error estimates can inform surrogate construction ameliorating these problems.

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MS92

Source Parameter Estimation For Volcanic Ash Transport and Dispersion Using Polynomial Chaos Type Surrogate Models

We present a framework for probabilistic volcanic ash plume forecasting using an ensemble of simulations, guided by Conjugate Unscented Transform (CUT) method for evaluating integrals. This ensemble is used to construct a polynomial chaos expansion that can be sampled cheaply, to either provide a forecast or combined with a minimum variance condition, to provide a full posterior pdf of the uncertain source parameters, based on observed satellite imagery.

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MS93

Learning About Physical Parameters: the Importance of Model Discrepancy

We illustrate through a simple example that calibration without account for model discrepancy (model error) may lead to biased and over-confident parameter estimates and predictions. Incorporating model discrepancy is difficult since it is confounded with calibration parameters, which will only be resolved with meaningful priors. For our simple example, we model the model-discrepancy via a Gaussian process and demonstrate that our prediction within the range of data is correct, but only with realistic priors on the model discrepancy do we uncover true parameter values.

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MS93

Bayesian Estimates of Model Inadequacy in Reynolds-Averaged Navier-Stokes

Errors due to turbulence modeling are the only uncontrolled source of error in RANS simulations of perfect gases. We compare two recently proposed methods for estimating turbulence modeling errors, based on model coefficient and model-form uncertainty. We examine their accuracy in several high Reynolds number flows, and compare the

resulting error estimates to discretization error. The goal is a better understanding of mesh-resolution requirements in RANS simulations.

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MS93

A Bayesian Viewpoint to Understanding Model Error

When combining massive data sets with complex physical models, one has to take into account "model error". We consider the problem of state prediction under an imperfect model, using a Bayesian approach. The underlying process is an advection-diffusion equation. Our results show that the prediction ability of a simple working model is increased significantly when accounting for model error, even though the right dynamics are not captured.

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MS93

Density Estimation Framework for Model Error Quantification

The importance of model error assessment during physical model calibration is widely recognized. We highlight the challenges arising in conventional statistical methods accounting for model error, and develop a density estimation framework to quantify and propagate uncertainties due to model errors. The reformulated calibration problem is then tackled with Bayesian techniques. We demonstrate the key strengths of the method on both synthetic cases and on a few practical applications.

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MS94

Multilevel Drift-Implicit Tau Leap

In biochemical reactive systems with small copy numbers of one or more reactant molecules, stochastic effects are often dominant. In such systems, those characterized by having simultaneously fast and slow time scales, the existing discrete space-state stochastic path simulation methods such as the stochastic simulation algorithm (SSA) and the explicit tau-leap method can be very slow. In this work, we propose a fast and efficient Multilevel Monte Carlo method that uses drift-implicit tau-leap approximations.

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MS94

MLMC for Multi-Dimensional Reflected Diffusions

The talk will discuss the combination of adaptive time stepping with multilevel Monte Carlo (MLMC) applied to multi-dimensional reflected diffusions. By refining the timestep as the path approaches the boundary, the accuracy is significantly improved for a given computational cost per path. Overall, it is possible to achieve a root-mean-square accuracy of ε for a computational cost which is $O(\varepsilon^{-2})$, and could potentially be further improved by using multilevel quasi-Monte Carlo methods. Both numerical results and supporting numerical analysis will be presented.

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MS94

Monte Carlo Methods and Mean Field Approximation for Stochastic Particle Systems

I discuss using single level and Multilevel Monte Carlo (MLMC) methods to compute quantities of interests of a stochastic particle system in the mean-field. In this context, the stochastic particles follow a coupled system of Ito stochastic differential equations (SDEs). Moreover, this stochastic particle system converges to a stochastic mean-field limit as the number of particles tends to infinity. In this talk, I start by recalling the results that first appeared in (Haji-Ali, 2012) where I developed different versions of MLMC for particle systems, both with respect to time steps and number of particles and proposed using particle antithetic estimators for MLMC. In that work, I showed moderate savings of MLMC compared to Monte Carlo. Next, I expand on these results by proposing the use of our recent Multi-index Monte Carlo method to obtain improved convergence rates.

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MS94

Multilevel Monte Carlo Approximation of Quantiles

The multilevel Monte Carlo method has been established as a computationally efficient sampling method for approximating moments of uncertain system outputs. Its use for statistical objects that cannot be expressed as moments, however, has not yet received much attention. An example of such an object is the quantile, which has become an integral part in many applications, such as in robust optimization. In this talk we discuss multilevel Monte Carlo techniques allowing a quantile estimation.

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MS95

High Dimensional Bayesian Optimization Via Random Embeddings Applied to Automotive Design

Bayesian optimization using random embeddings has been shown to efficiently deal with high number of variables under the assumption that only a few of them actually are influential. We discuss in particular the choice of the random matrix defining the linear embedding and of the covariance kernel for the Gaussian process surrogate model. We further adapted the method to deal with a test case in car crash-worthiness in constrained and multi-objective optimization setups.

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MS95

Multi-Objective Bayesian Optimization: Calibrating a Tight Gas Condensate Well in Western Canada

The history matching process of physical high dimensional models is a costly task. We apply Gaussian Processes for both single-objective and multi- objective calibration using real multi-stage horizontal gas condensate well data from the Montney Formation in Western Canada. The results show a quick convergence in less than 100 simulations for this 20-dimensional problem. The resulting Pareto front showed a quick convergence with a good match quality in less than 200 simulations.

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MS95

Scalable Bayesian Optimization

Bayesian optimization is an effective approach to find the global extremum of functions that are expensive to evaluate. In this work we propose a scalable parallelization of this technique that outperforms, in wall-clock time, previous results in the literature. A new open source python framework, GPyOpt, with an efficient implementation of this and other Bayesian optimization techniques is also presented as a complement to our work.

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MS96

A Variational Bayesian Sequential Monte Carlo Filter for Large-Dimensional Systems

This work considers the Bayesian filtering problem in high-dimensional nonlinear state-space systems for which classical Particle Filters (PFs) are impractical due to the prohibitive number of required particles to obtain reasonable performances. To deal with the curse of dimensionality, we resort to the variational Bayesian approach to split the state-space into low-dimensional subspaces, and subsequently apply one PF to each subspace. The propagation of each particle in the resulting filter requires generating one particle only, in contrast with the existing multiple PFs for which a set of (children) particles needs to be generated. After describing the proposed filter, we present numerical results to evaluate its behavior and to compare its performances against the standard PF and a multiple PF.

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MS96

Forward Backward Doubly Stochastic Differential Equations and the Optimal Filtering of Diffusion Processes

Abstract not available.

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MS96

Filtering Compressible and Incompressible Turbulent Flows with Noisy Lagrangian Tracers

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MS96

Efficient Assimilation of Observations Via a Localized Particle Filter in High-Dimensional Geophysical Systems

We introduce a localized particle filter (PF) that has potential for high-dimensional data assimilation applications in geoscience. Unlike standard PFs, the local PF uses a tapering function to reduce the influence of observations on weights needed for approximating posterior probabilities, thus decreasing the number of particles required to prevent filter divergence. The local PF and ensemble Kalman filters are compared in atmospheric models to demonstrate benefits of the new method over linear filters.

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MS97

Ordering Heuristics for Minimal Rank Approximations in Tensor-Train Format

The efficiency of the tensor-train (TT) decomposition of tensors resulting from the discretization of multidimensional functions relies on the existence of low-rank approximations of different unfoldings. The order in which the associated dimensions are considered can lead to dramatically different TT-ranks, however, and thus deteriorate the compression level (which scales quadratically with the ranks). We will present heuristics which can be used to find improved orderings for TT approximation, at the expense of some limited pre-processing costs.

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MS97

Adapted Tensor Train Approximations of Multivariate Functions Using Least-Squares Methods

We propose low-rank tensor train (TT) approximation methods using least squares methods for the approximation of a multivariate function from random, noisy-free observations. Here we present different algorithms for the construction of the tensor train approximations, based either on density matrix renormalization group (DMRG) or alternating least squares (ALS) methods, that are designed so to provide adaptation of the rank and adaptation of the univariate bases.

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MS97

Low-Rank Tensor Approximations for the Computation of Rare Event Probabilities

Rare-event simulation with complex high-dimensional computational models remains a challenging problem. This work demonstrates that meta-models belonging in the class of low-rank tensor approximations can provide an accurate representation of the PDF of the model response at the tails, thus leading to efficient estimation of rare-event probabilities. Because the number of unknowns in such meta-models grows only linearly with the input dimension, high-dimensional problems are addressed by relying on relatively small experimental designs.

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MS97

Low Rank Approximation-Based Quadrature for Fast Evaluation of Quantum Chemistry Integrals

A new method based on low rank tensor decomposition for fast evaluation of high dimensional integrals in quantum chemistry is proposed. The integrand is first approximated in a suitable low rank canonical tensor subset with only a

few integrand evaluations using classical alternating least squares. This allows representation of a high dimensional integrand function as sum of products of low dimensional functions. In the second step, low dimensional Gauss Hermite quadrature rule is used to integrate this low rank representation thus avoiding the curse of dimensionality. Numerical tests on water molecule demonstrate the accuracy of this method using very few samples as compared to Monte Carlo and its variants.

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MS98

Multilevel Sequential Monte Carlo Samplers

Sequential Monte Carlo (SMC) samplers are a popular and versatile class of algorithms for computationally intensive inference problems. One constructs a sequence of intermediate distributions and associated Markov chain kernels such that sequential importance sampling and resampling can guide the samples to the regions of high probability, hence avoiding degeneracy of the weights and explosion of the variance. For problems which admit a hierarchy of approximation levels, the multilevel Monte Carlo (MLMC) sampling framework enables a reduction of cost by leveraging a telescopic sum of increment estimators with vanishing variance. These ideas can be combined in a very natural way to yield the MLSMC sampling algorithm for Bayesian inverse problems. The theoretical results will be illustrated by a numerical example of permeability inversion through an elliptic PDE given observations of the pressure

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MS98

Metropolis-Hastings Algorithms in Function Space for Bayesian Inverse Problems

We consider Markov Chain Monte Carlo methods adapted to a Hilbert space setting. Such algorithms occur in Bayesian inverse problems where the solution is a probability measure on a function space according to which one would like to integrate or sample. We focus on Metropolis-Hastings algorithms and, in particular, we introduce and analyze a generalization of the existing pCN-proposal. This new proposal allows to exploit the geometry or anisotropy of the target measure which in turn might improve the statistical efficiency of the corresponding MCMC method. In numerical experiments resulting methods displayed superior statistical efficiency to pCN and behaves robustly with respect to dimension and noise variance.

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MS98

Multilevel Markov Chain Monte Carlo Method for Bayesian Inverse Problems

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MS98

Accelerating Metropolis Algorithms Using Transport Maps

We present a new approach for efficiently characterizing complex probability distributions, using a combination of optimal transport maps and Metropolis corrections. We use continuous transportation to transform typical Metropolis proposal mechanisms into non-Gaussian proposal distributions. Our approach adaptively constructs a Knothe-Rosenblatt rearrangement using information from previous MCMC states, via the solution of convex and separable optimization problems. We then discuss key issues underlying the construction of transport maps in high dimensions, and present ways of exploiting sparsity and low-rank structure.

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MS99

Solver- vs. Grid-Hierarchies for Multi-Level Monte Carlo Sampling of Subsurface Flow and Transport

For fast sampling in the context of PDEs, multilevel Monte Carlo (MLMC) combines traditionally a multigrid technique with Monte Carlo (MC) sampling. In our work, we apply instead of grids of different resolution a hierarchy

of solution methods of different accuracy. In the context of two-phase flow and transport, we demonstrate that the resulting solver MLMC leads like traditional MLMC to significant speedups while offering greater flexibility in certain applications.

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MS99

Reduced Hessian Method for Uncertainty Quantification in Ocean State Estimation

Reduced rank Hessian-based method for quantifying uncertainty covariance in ocean state estimation is implemented by direct second order Algorithmic Differentiation of a nonlinear General Circulation Model. Dimensionality of the least-squares misfit Hessian inversion is reduced by omitting its nullspace, as an alternative to suppressing it by regularization, excluding from the computation the uncertainty subspace unconstrained by observations. Inverse and forward uncertainty propagation schemes are designed for assimilating observation uncertainty and evolving it through the model.

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MS99

Detecting Low Dimensional Structure in Uncertainty Quantification Problems

Detecting low dimensional structure is useful for the uncertainty quantification for complex systems as it captures the main property of the system. We propose a method to achieve this goal by combining the active subspace and the compressive sensing method. With several iterations, this approach is able to detect important dimensions which are linear combination of the original parameters. We use PDEs and a biomolecular system to demonstrate the efficiency of this method.

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MS99

Speeding Up Variational Inference

Four dimensional variational (4D-Var) approach formulates data assimilation as an optimization problem and computes a maximum aposteriori estimate of the initial condition and parameters of the dynamical system under consideration. The solution of large 4D-Var problems poses considerable challenges: the construction and validation of an adjoint model is an extremely labor-intensive process; strong-constraint 4D-Var is computationally expensive; and 4D-Var does not include posterior uncertainty estimates. In this talk we present several ideas to tackle these challenges: performing efficient computations using reduced order model surrogates, exploiting time parallelism, and constructing smoothers that sample directly from the posterior distribution.

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MS100

Bayesian Filtering in Cardiovascular Models

Uncertainty quantification plays an important role in modeling cardiovascular dynamics, especially in rendering physiological models patient-specific for use in clinical decision-making, where it is essential to determine output uncertainty. Given experimental data and models with numerous sources of uncertainty, such as the underlying, perhaps time-varying system parameters, we show how Bayesian filtering techniques can be employed in this setting to estimate unknown model states and parameters, providing a natural measure of uncertainty in the estimation.

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MS100

Sparse Mode Decomposition for High Dimensional Random Fields, and Its Application on Spde

Inspired by the recent developments in data sciences, we introduce an intrinsic sparse mode decomposition method for high dimensional random fields. This sparse representation of the random field allows us to break a high dimensional stochastic field into many spatially localized modes with low stochastic dimension locally. Such decomposition enables us to break the curse of dimensionality in our local solvers. To obtain such representation, we first decompose the covariance function into low part plus sparse parts. We then extract the spatially localized modes from the sparse part by minimizing a surrogate of the total area of the support. Moreover, we provide an efficient algorithm to solve it. As an application, we apply our method to solve elliptic PDEs with random media having high stochastic dimension. Using this localized representation, we propose various combinations of local and global solver that achieve different level of accuracy and efficiency. At the end of the talk, I will also discuss other applications of the intrinsic sparse mode extraction. This work is in collaboration with Thomas Y. Hou and Pengchuan Zhang.

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MS100

Efficient Evaluation of Hessian Operators Arising in Large-scale Inverse Transport Problems

Recent developments in infinite-dimensional Bayesian inverse problems with PDE constraints have demonstrated that an efficient evaluation of the Hessian operator is critical. Sampling the associated high-dimensional probability density functions has only recently become feasible. Hessian based proposals can be used to guide the sampler to regions with higher acceptance probability. Applications that drive our research are in medical imaging with a number of unknowns that, upon discretization, is in the millions or billions. Explicitly constructing the Hessian is therefore out of question, not only due to memory requirements, but also because it requires one expensive forward and adjoint PDE solve per unknown. Our solver operates in a deterministic setting; it provides a MAP point estimate. We will describe efficient ways for evaluating the Hessian operator and discuss ideas for its approximation based on problem specific preconditioners for the associated reduced space KKT system. We will see that the optimality systems are multiphysics systems of nonlinear, multicomponent PDEs, which are challenging to solve in an efficient way. We will showcase convergence and scalability results of our solver for 3D synthetic and real-world problems of varying complexity.

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MS100

A Hierarchical Bayesian Approach to Pharmacokinetics Study

Pharmacokinetic models consist of a large set of ordinary differential equations with many model parameters and large uncertainties. We introduce a hierarchical Bayesian framework to account for the model parameters uncertainty across patients using a case study of brain tumor treatment. This uncertainty is explicitly separated from the typical additive noise that represents other model uncertainties and measurement noise. We present an efficient approximation method to handle the intensive computations required by the hierarchical model.

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MS101

Uncertainty Quantification for Complex Multiscale Systems

Multiscale modeling efforts must adequately quantify the effect of both parameter uncertainty and model discrepancy across scale. Advancements in uncertainty quantification using Bayesian calibration are described; a dynamic discrepancy approach to upscale uncertainty, functional inputs and extrapolation uncertainty, and a large parameter space. For emulation and discrepancy modeling, a Bayesian Smoothing Spline ANOVA (BSS-ANOVA) approach is utilized. These approaches are applied here to applications in chemical kinetics and carbon capture technology, with wide ranging impact.

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MS101

Solving Stochastic Elliptic Boundary Value Problems with a Multis-Scale Domain Decomosition Method

In subsurface flow models quantifying uncertainty of coefficients which have multiple scales of heterogeneity presents a challenge. Typically, Monte-Carlo methods have been used to model this uncertainty. Separately, multiscale finite element methods have been developed to accurately capture heterogeneous effects of spatial heterogeneity. Since the heterogeneity of individual realizations can differ drastically, a direct use of multiscale methods in Monte-Carlo simulations is problematic. Furthermore, Monte-Carlo methods are known to be very expensive as a lot of samples are required to adequately characterize the random component of the solution. In this study, we utilize a stochastic representation method that exploits the solution structure of the random process in order to construct a problem dependent stochastic basis. Using this stochastic basis representation a set of coupled yet deterministic equations can be constructed. To reduce the computational cost of solving the coupled system, we develop a Multi-Scale Domain Decomposition method which utilizes Robin transmission conditions. In the developed Multi-scale method enrichment of the Multi-Scale solution space can be performed at multiple levels offering a balance between computational cost, and accuracy of the found solution.

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MS101

Balancing Sampling and Discretization Error in the Context of Multi-Level Monte Carlo

Multilevel Monte Carlo (MLMC) involves two types of errors: a sampling and a discretization error. In this work, we present an error balancing strategy that follows an optimal total error vs. total work decay. We estimate the two errors on the fly based on power law assumptions. For testing, we consider two-phase flow and transport in a heterogeneous porous media and find growing performance gains for an increasing number of MLMC levels.

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MS101

Uncertainty Quantification in Cloud Cavitation Collapse Using Multi-Level Monte Carlo

Cloud cavitation collapse pertains to the erosion of liquid-fuel injectors, hydropower turbines, ship propellers, and is harnessed in shock wave lithotripsy. To assess the development of extreme pressure spots, we performed numerical two-phase flow simulations of cloud cavitation collapse containing 50’000 bubbles using 1 trillion cells. To quantify the uncertainties in the collapsing clouds under random initial conditions, we investigate a novel non-intrusive multi-level Monte Carlo methodology, aiming to accelerate the plain Monte Carlo sampling.

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MS102

Sparse Approximation of Elliptic PDEs with Lognormal Coefficients

We consider elliptic partial differential equations with diffusion coefficients of lognormal form. For such problems, we study the ℓ^p-summability properties of the Hermite polynomial expansion of the solution in terms of the countably many scalar parameters in the representation the random field. Our estimates significantly improve on known results, with direct implications on the approximation rates of best n-term Hermite expansions.

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MS102

High-Dimensional Approximation Using Equilibrium Measures

We consider the problem of approximating solutions to parameter-dependent partial differential equations. Standard approaches frequently involve collecting PDE solutions computed at a judiciously-chosen finite set of parametric samples, and using these to predict the solution manifold behavior for all parameter values. In this talk we consider choosing parameter samples according to the pluripotential equilibrium measure. We also show that such an approach typically yields very stable, high-order computational procedures for parametrized PDE approximation.

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MS102

Smoothing by Integration and Anova Decomposition of High-Dimensional Functions

In recent joint papers with Michael Griebel and Frances Kuo we have shown that the lower ANOVA terms of a non-smooth function can be smooth, because of the smoothing effect of integration. The problem settings have included both the unit cube and the Euclidean space, and in the latter case even infinite-dimensional integration. The talk will survey this work, and report on recent developments.

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MS102

Title Not Available

Abstract not available.

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MS103

A Data-Driven Approach to PDE-Constrained Optimization Under Uncertainty

PDE-constrained optimization problems often possess uncertain coefficients, boundary data, etc. In many applications, the probabilistic characterization of these uncertainties is unknown and must be estimated using data. I present an approach to incorporate data in such problems using distributionally robust optimization. First, I discuss theoretical properties concerning distributionally robust PDE-optimization. Then, I introduce a novel data-driven discretization with rigorous error bounds for the unknown probability measure. I conclude with numerical results.

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MS103

Multidimensional Buffered Probability of Exceedance and Applications to Distribution Approximation

Probability of exceedance (POE) is widely used but has major drawbacks. Buffered probability of exceedance (bPOE) is a conservative approximation of POE, eliminating some of its drawbacks. We suggest a new multi-dimensional generalization of bPOE (M-bPOE) to control exceedances for several random variables simultaneously. Distribution approximation problems with M-bPOE constraints are studied. Entropy maximization with M-bPOE dominance, which unifies convex-linear second order and lift zonoid dominances, and variance constraints leads to maximum-of-Gaussians form of optimal solution.

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MS103

Buffered Probability of Exceedance, Support Vector Machines, and Robust Optimization

We first present a new probabilistic characteristic, called Buffered Probability of Exceedance (bPOE) and show that bPOE acts as a natural counterpart to Probability of Exceedance (POE), but with superior mathematical properties, in particular leading to convex optimization problems. Turning to application of bPOE, we then show that the famous Support Vector Machine's (SVM's) used for binary classification are equivalent to simple bPOE minimization, providing a new purely probabilistic interpretation of SVM's. We then show that this relationship reveals a connection between bPOE minimization and Robust Optimization (i.e. deterministic optimization over fixed uncertainty sets).

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MS103

Gas Transportation under Stochastic Uncertainty: Nomination Validation and Beyond

For steady-state gas networks with uncertain outlets probabilities of validity are computed for balanced nominations. The mathematical modeling follows Kirchhoff's Laws. Placing accent on passive networks the role of fundamental cycles is highlighted from analytic as well as algebraic perspectives. Structural information acquired this way turns out beneficial when applying Quasi Monte Carlo Sampling for the calculation of the desired probabilities.

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MS104

Combined Reduction for Uncertainty Quantification

Often, uncertainty quantification tasks practically amount to a many-query setting, like model-constraint optimization; and realistic input-output models are of large-scale and contain many uncertain parameters. Hence, a swift repeated evaluation usually requires model order reduction. Combined reduction is a parametric model reduction technique that concurrently approximates the dominant state- and parameter-space. The reduced order model then accelerates the single simulation, and the low-rank approximation to the original high-dimensional parameter-space the overall task.

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MS104

Multifidelity Methods for Uncertainty Quantification

Replacing high-fidelity models with low-cost surrogate models to accelerate sampling-based UQ usually leads to biased estimates, because the surrogate model outputs are only approximations of the high-fidelity model outputs. We introduce multifidelity methods that combine, instead of replace, the high-fidelity model with surrogate models. An optimization problem balances the number of model evaluations among the models to leverage surrogate models for speedup. Recourse to the high-fidelity model provides guarantees of unbiased estimates in the statistics of interest.

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MS104

Error Estimates for Reduced-Order Models Using Statistical Learning

We present a statistical learning framework for estimating the error introduced by reduced-order models (ROMs) applied to nonlinear dynamical systems. We use statistical techniques for high-dimensional regression to map a large set of inexpensively-computed quantities (generated by the time-dependent ROM) to errors in the output quantities of interest. We demonstrate the procedure on a trajectory piecewise linear (TPWL) ROM applied to subsurface oil-water flow problems with varying well-control parameters.

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MS104

Adaptive Stochastic Collocation for PDE-Constrained Optimization under Uncertainty using Sparse Grids and Model Reduction

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 (with statistically quantified errors) 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.

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MS105

Rare Event Computation and Large Deviation for Geophysical Turbulent Flows and Climate Applications

Abstract not available.

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MS105

Singularities, Instantons and Turbulence

It is evident that coherent nearly singular structures play a dominant role in understanding the anomalous scaling behavior in turbulent systems. We ask the question, which role these singular structures play in turbulence statistics. More than 15 years ago, for certain turbulent systems the door for attacking this issue was opened by getting access to the probability density function to rare and strong fluctuations by the instanton approach. We address the question whether one can identify instantons in direct numerical simulations of the stochastically driven Burgers equation. For this purpose, we first solve the instanton equations using the Chernykh Stepanov method [2001]. These results are then compared to direct numerical simulations by introducing a filtering technique to extract prescribed rare events from massive data sets of realizations. In addition, we solve the issue why earlier simulations by Gotoh [1999] were in disagreement with the asymptotic prediction of the instanton method and demonstrate that this approach is capable to describe the probability distribution of velocity differences for various Reynolds numbers. Finally, we will present and discuss first results on the instanton solution for vorticity in 3D Navier Stokes turbulence.

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MS105

A Minimum Action Method for Navier-Stokes Equations Based on a Divergence-Free Basis

Abstract not available.

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MS105

Gentlest Ascent Dynamics for Locating Transition States

Transition state is of critical importance to describe the rare event in escaping an attractor. Most of time, these states are of saddle point type. In this talk, we review the numerical methods of locating transition state or the saddle point both on an energy landscape and for non-gradient dynamics. These include joint work with Weinan E (Peking University and Princeton University) and Weiguo Gao, Jing Leng (Fudan University).

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MS106

Probability Models for Discretization Uncertainty and Adaptive Mesh Selection

Abstract not available.

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MS106

Uncertainty Quantification with Gaussian Process Latent Variable Models

Stochastic analysis of multiscale problems requires a realistic data-driven stochastic model of the material property variations. In this work, we use the Gaussian Process latent variable model (GP-LVM), a kernel based method that provides a probabilistic mapping from the latent space to the physical property space. We examine the performance of the method in dimensionality reduction of multiscale properties and use it with a multi-output sparse GP model for uncertainty propagation in multiphase flows.

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MS106

Lightweight Error Estimation, Using the Probabilistic Interpretation of Classic Numerical Methods

Certain classic numerical methods for integration, linear algebra, optimization, and the solution of differential equations construct least-squares approximations for non-analytic quantities from computable ones, and can thus be directly interpreted as Bayesian maximum a-posteriori (mean) estimators under a number of structured Gaussian priors. With a particular focus on solvers for ordinary differential equations, I will discuss approaches for the calibration of the covariance of the associated Gaussian posterior at runtime, which endow these classic methods with error estimates expressed as probability measures. The emphasis will be on computationally lightweight implementations of this type of error estimation. If time permits, I will also discuss some recent applications.

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MS107

Structural Discrepancy Analysis for Natural Hazards Models

Structural discrepancy refers to the differences between a computer simulator and the physical system that the simulator purports to represent, even when the simulator is evaluated at appropriate choices of input parameters. Careful assessment of structural discrepancy is essential when considering the relevance of a simulator for decisions concerning the physical system. We will discuss how such such discrepancy may be assessed and utilised, paying particular attention to features related to internal discrepancy, i.e. those features of structural discrepancy that may be assessed directly by means of experiments on the computer simulator. The approach will be illustrated by examples in flood modelling.

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MS107

Coupling Computer Models Through Linking

Their Statistical Emulators

Direct coupling of computer models is often difficult for computational and logistical reasons. We propose coupling two computer models by linking independently developed Gaussian process emulators (GaSPs) of these models. The linked emulator results in a smaller epistemic uncertainty than a direct GaSP of the coupled computer model would have (if such a model were available). This feature is illustrated via simulations. The application of the methodology to complex computer models is demonstrated as well.

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MS107

Multi-Objective Sequential Design for Computer Experiments

Using a combination of statistical emulators and a modified version of the EGO (Efficient Global Optimization) algorithm, we conduct a search of a state space for design points that are of relevance for emulators of simulator output at multiple physical locations simultaneously. This sequential design methodology reduces the number of expensive model runs to be made and is used to generate probabilistic hazard maps of inundation due to volcanic landslides (pyroclastic flows).

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MS107

Developing a Shallow-Layer Model of Lahars for Hazard Assessment

Lahars are highly concentrated mixtures of mobilized volcanic material that are potentially extremely destructive to populations living around volcanoes. We present a new predictive model of lahars that can describe a variety of flow regimes from concentrated streamflows to lubricated granular flows. We explore different parameterisations for erosion/deposition and basal drag, compare their uncertainty with that in model forcing, and demonstrate the use of emulation to facilitate efficient model evaluations and therefore rapid hazard assessment.

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MS108

Uncertainty in Modeling Turbulence: Data Inference and Physics Constraints

Turbulence models are commonly used in simulations of engineering flows. We investigate the the effect of modeling assumptions built in the models using perturbation analysis applied to the Reynolds stress definition. Furthemore we use machine learning techniques to identify the impact of specific closures on the predictions. Applications include aerodynamic flows in internal passages.

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MS108

Multi-Response Approach to Improving Identifiability in Model Calibration

One of the main challenges in model calibration is the difficulty in distinguishing between the effects of calibration parameters versus model discrepancy. A multi-response approach is developed to improve identifiability by using multiple responses that share a mutual dependence on a common set of calibration parameters. To address the issue of how to select the most appropriate set of responses to measure experimentally to best enhance identifiability, a preposterior analysis approach is developed and a surrogate preposterior analysis is employed to enhance the computational efficiency of the approach.

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MS108

Assessing Model Error in Reduced Chemical Mechanisms

In the field of combustion, reduced chemical mechanisms are often used because the detailed model is unknown or too computationally expensive. However, introducing a reduced model can be a significant source of model error. We represent this error with an operator that is both probabilistic and physically meaningful. The distributions of the operator are calibrated using high-dimensional hierarchical Bayesian modeling. We apply the stochastic operator method to various combustion mechanisms and investigate its effects on a one-dimensional laminar flame.

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MS108

Uncertainty Due to Inadequate Models of Scalar Dispersion in Porous Media

We present recent developments on the uncertainty quantification of models. Models are an imperfect representation of complex physical processes, hence exploring representations of the model inadequacies is crucial. We introduce a novel Bayesian framework for capturing the inadequacy in the context of a linear operator acting on the model solution. This framework is applied to predicting breakthrough curves with uncertainty in the context of scalar dispersion in porous media, but is applicable to other models.

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MS109

An Optimized Multilevel Monte Carlo Method

In many textbooks one of the first simple applications of the classical Monte Carlo method is Buffon's needle problem, where for a given length of a needle one is interested in the probability of the event that when thrown the needle hits one of some parallel lines. If one interprets the length of the needle as a free parameter one can also apply a multilevel Monte Carlo algorithm in order to approximate the hitting probabilities for all admissible parameter values simultaneously. It turns out that for this problem the exact solution, the statistical bias, the computational effort and all variances can be computed explicitly. This allows us to given sharp lower and upper estimates of the complexity of the multilevel Monte Carlo algorithm for this problem.

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MS109

Multilevel Subset Simulation for Rare Events

In subset simulation (Au & Beck, 2001), rare events are expressed as products of larger conditional failure sets. In our new multilevel approach, the conditional probabilities are estimated using different model resolutions. Most samples are computed on the coarsest grid, leading to efficiency gains of more than an order of magnitude. The key is a posteriori error estimation which guarantees the critical subset property that may be violated when changing model resolution between failure sets.

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MS109

Mean Square Adaptive Mlmc for Sdes

We present a formal mean square error (MSE) expansion for numerical solutions of stochastic differential equations (SDE). The expansion is used to construct an adaptive Euler–Maruyama algorithm for SDEs. The resulting algorithm is incorporated into a multilevel Monte Carlo (MLMC) algorithm. This novel algorithm is particularly efficient in solving low-regularity problems, outperforming uniform time-stepping MLMC and producing errors bounded with high probability by TOL at a cost rate $\mathcal{O}(TOL^{-2}\log(TOL)^4)$.

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MS110

Adaptive Design of Experiments for Conservative Estimation of Excursion Sets

We consider a Gaussian process model trained on few evaluations of an expensive to evaluate deterministic function and we study the problem of estimating a fixed excursion set of this function. We focus on conservative estimates of the excursion set and we present a method based on Vorob'ev quantiles, that sequentially selects new evaluations of the function in order to reduce the uncertainty on

the estimate. The method is then applied to a test case.

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MS110

Bias and Variance in the Bayesian Subset Simulation Algorithm

The Bayesian Subset Simulation (BSS) algorithm is a recently proposed approach, based on Sequential Monte Carlo simulation and Gaussian process modeling, for the estimation of the probability that $f(X)$ exceeds some thresold u when f is expensive to evaluate and $P(f(X) > u)$ is small. We discuss in this talk the bias an variance of the BSS algorithm, and propose a variant where the bias-variance trade-off is automatically tuned.

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MS110

Stepwise Uncertainty Reduction Strategies for Inversion of Expensive Functions with Nuisance Parameters

We deal with sequential evaluation strategies of real-valued, expensive, functions f in the context where the input parameters consist of controlled parameters and some nuisance, uncontrolled, parameters. Mathematically, we identify all controlled parameters $\{x_c : \forall x_n \; f(x_c, x_n) < T\}$ where f does not have any failure whatever the value of the nuisance parameters. A sampling criterion relying on recent kriging update formulas is used and applied to a nuclear safety test case.

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MS110

Sequential Design for the Estimation of High-Variation Regions Using Differentiable Non-Stationary Gaussian Process Models

Gaussian Process models have proven useful for sequential design of computer experiments. Here we focus on the case of functions possessing heterogeneous variations across the input space. We propose two sequential design approaches dedicated to learning high variation regions: devising derivative-based infill criteria or using standard ones under ad hoc non-stationary GP models. We compare the advantages of both methods based on a benchmark of simulated functions and on the motivating mechanical engineering test case.

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MS111

On Probabilistic Transformations and Optimal Sampling Rules for Emulator Based Inverse UQ Problems

The efficiency of all generalized polynomial chaos expansion based methods decrease significantly if the model inputs are dependent random variables. This talk will discuss probabilistic transformations such as the Rosenblatt and the Nataf transformation that decorrelate random variables for improving the efficiency of Bayesian inverse problems. We will present numerical studies that demonstrate the effectiveness of these transformations and present some alternatives such as leja sequences in combination with arbitrary polynomial chaos expansion.

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MS111

Probabilistic Inference of Model Parameters and Missing High-Dimensional Data Based on Summary Statistics

We present a method based on Maximum Entropy and Approximate Bayesian Computation for probabilistic inference of combustion system parameters from indirect summary statistics. The approach relies on generating high-dimensional data consistently with the given statistics. Importance sampling and Gauss-Hermite quadrature are used for parameter inference. Nuisance parameters with prescribed marginal posterior probability density are addressed. A consensus joint posterior on the parameters is obtained by pooling the posterior parameter densities given the consistent data sets.

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MS111

Incomplete Statistical Information Limits the Utility of Higher-Order Polynomial Chaos Expansions

Polynomial chaos expansion is a well-established massive stochastic model reduction technique that approximates the dependence of model output on uncertain input parameters. In practice, only incomplete and inaccurate statistical knowledge on uncertain input parameters is available. Observation of the expansion convergence when statistical input information is incomplete demonstrates that higher-order expansions without adequate data support are useless. We offer a simple relation that helps to align available input statistical data with an adequate expansion order.

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MS111

Adaptive Response Surface Approximations for Bayesian Inference

While the most popular technique for stochastic inference is the statistical Bayesian approach, a new approach based on measure-theoretic principles has emerged in recent years. In this presentation, we discuss how Bayesian concepts can be applied within the measure-theoretic framework to develop a new approach for Bayesian inference. We then show how adaptive surrogate models can be employed with the specific objective of adapting the response surface to accurately perform stochastic inversion.

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MS112

Deep Learning for Multiscale Inverse Problems

A Bayesian computational approach is developed to estimate spatially varying parameters in a multiscale inverse problem. The spatial field is re-parameterised using a sparse adaptive wavelet representation, forming a deep network between the wavelet coefficients at different levels. A sequential Monte Carlo sampler is used to explore the posterior distribution of the wavelet coefficients at each level. The method is demonstrated with the estimation of a multiscale permeability field in fluid flows through porous media.

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MS112

Anova Based Reduced Basis Methods for Partial Differential Equations with High Dimensional Random Inputs

Abstract not available.

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MS112

Parallel Implementation of Non-Intrusive Stochastic Galerkin Method for Solving Stochastic Pdes

In multi-parametric equations - stochastic equations are a special case - one may want to approximate the solution such that it is easy to evaluate its dependence of the parameters. Very often one has a "solver" for the equation for a given parameter value - this may be a software component or a program - it is evident that this can independently solve for the parameter values to be interpolated. Such uncoupled methods which allow the use of the original solver are classed as "non-intrusive". By extension, all other methods which produce some kind of coupled system are often - in our view prematurely - classed as "intrusive". We showed in for simple Galerkin formulations of the multi-parametric problem how one may compute the approximation in a non-intusive way. Now we extend the results presented in by implementing a parallel version of numerical methods.

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MS113

Affine Invariant Samplers for Bayesian Inverse Problems

Abstract not available.

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MS113

Asymptotic Analysis of Random-Walk Metropolis on Ridged Densities

The asymptotic behavior of local-move MCMC algorithms in high-dimensions is by now well understood and the emergence of diffusion processes as trajectory limits has been proved in many such contexts. The results obtained so far involve mainly i.i.d scenarios, though there are now a number of generalizations in high/infinite dimensions. We adopt a different point of view and look at cases when the target distributions tend to exhibit 'ridges' along directions of the state space. Such contexts could arise for instance in classes of models when data arrive with small noises or when there are non-identifiable subsets of parameters. In an asymptotic context all probability mass will concentrate on a manifold. We show that diffusion limits (on a manifold) abound also in this set-up of ridged densities and are particularly useful for identifying computational costs or providing optimality criteria.

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MS113

Analysis and Optimization of Stratified Sampling

Stratified sampling methods compute averages over a target distribuion by partitioning the sample space into subregions, sampling conditional distributions confined to the subregions, and computing averages over the target distribution from the conditional averages. Such methods may be used to compute both averages with respect to the ergodic measure of a process and also dynamical quantities, such as reaction rates, of interest in molecular simulation. We analyze the benefits of stratified sampling, and we discuss some techniques for optimizing the parameters involved in the method.

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MS113

An Analytical Technique for Forward and Inverse Propagation of Uncertainty

Sampling methods for forward (Monte Carlo) and inverse (Markov Chain Monte Carlo) propagation of uncertainty involving complex models remain a computationally extremely challenging task. In this talk, we consider a quadratic approximation of the quantity of interest with respect to the stochastic parameter, for which – assuming a Gaussian prior distribution of the parameter – an analytical expression for the expected value is known. We then exploit such quadratic approximation as a variance reduction technique to accelerate the convergence of Monte Carlo and Markov Chain Monte Carlo sampling methods.

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MS114

Stochastic Representation of Model Inadequacy for

Supercapacitors

A probabilistic formulation of model inadequacy is developed for a reduced (upscaled) supercapacitor model. The errors introduced by modeling assumptions during upscaling are accounted for through injecting stochasticity into the reduced model equations. The mathematical formulation of the injected stochasticity is informed by spatio-temporal error estimates using residual information, which bypasses the need to solve higher-fidelity equations. The reliability of these stochastic representations is then examined using deterministic observations from a higher-fidelity supercapacitor model.

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MS114

Hierarchical Optimization for Neutron Scattering Problems

We present a scalable optimization method for neutron scattering problems that determines confidence regions of simulation parameters in lattice dynamics models used to fit neutron scattering data for crystalline solids. The method uses physics–based hierarchical dimension reduction in both the computational simulation domain and the parameter space. We demonstrate for silicon that after a few iterations the method converges to parameters values (interatomic force-constants) computed with density functional theory simulations.

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MS114

Uncertainty Quantification in Diffuse Optical Tomography

We consider efficient Bayesian inversion and uncertainty quantification for parameterized PDE-based inverse problems, such as Diffuse Optical Tomography. Although the parameterization reduces costs substantially, the spaces to be sampled remain high dimensional, say, hundreds to a thousand parameters. Hence, convergence of the posterior typically requires many samples, where each sample requires a large number of three-dimensional PDE solves. We discuss methods that reduce both the number of sample points as well as the computational effort per sample point in a complementary fashion.

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MS114

Reduction of Chemical Models under Uncertainty

We discuss recent developments for dynamical analysis and reduction of chemical models under uncertainty. We rely on computational singular perturbation analysis, allowing for uncertainties in reaction rate parameters. We outline a construction for representation of uncertain reduced chemical models, and estimation of probabilities for inclusion of sets of reactions in the reduced model. We demonstrate the approach in the context of homogeneous ignition of a hydrocarbon fuel-air mixture.

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MS114

Recursive k-d Darts Sampling for Exploring High-Dimensional Spaces

We introduce Recursive k-d Darts: a new hyperplane sampling algorithm to estimate statistical metrics (e.g., mean and tail-probability) of an underlying black-box high-dimensional function. Our method decomposes the high-dimensional problem into a set of 1-dimensional problems. This approach enables efficient handling of discontinuities and higher-order estimates in smooth regions. We quantify estimation errors by comparing a local and global surrogate models, built on the fly as sampling proceeds, and use that to guide future samples.

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MS115

Scalable Subsurface Characterization with Multiphysics Models and Massive Data Using Principal Component Geostatistical Approach

Bayesian Geostatistical approach is widely used for inverse problems in geosciences. However, the Jacobian matrix needs to be computed from $\mathcal{O}(\min(m, n))$ forward runs for m unknowns and n observations, which can be prohibitive when m and n become large with the advent of the era of "big' data. We present a scalable Jacobian-free inversion method and show the efficiency of the proposed method with arsenic-bearing mineral identification and massive MRI tracer data inversion examples.

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MS115

Bayesian Reconstruction of Catalytic Properties of Thermal Protection Materials for Atmospheric Reentry

Simulating the atmospheric entry of a spacecraft is a challenging problem involving complex physical phenomena, including the response of heatshield materials to extreme aerothermal conditions. Among others, the catalycity of the thermal protection material is extremely important since it quantifies the recombination of atoms at the surface, hence the heating transferred to the spacecraft. Using data from plasma testing, sources of uncertainty in the rebuilding of catalycity are identified and propagated through a Bayesian solver.

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MS116

Uncertainty Quantification for An Industrial Application

This contribution presents the application of uncertainty quantification to an electric drive from series production. The forward propagation is based on collocation methods using generalized polynomial chaos and the stochastic solution is verified by a test bench. Furthermore, the setup can be used for estimation of parameter distributions which are not known in general. The aim is to make uncertainty quantification applicable for a real use case in an electrical and mechanical engineering context.

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MS116

Numerical Methods for Uncertainty Propagation in Hybrid-dynamical Systems

Hybrid-dynamical systems often arise in context of mechatronic systems, parameters of which typically exhibit some level of uncertainty, due to, for example, incomplete knowledge. In this talk we evaluate the feasibility of the stochastic Galerkin projection using Polynomial Chaos for uncertainty propagation in a hybrid-dynamical benchmark problem with uncertain model parameters. A characteristic function approach is used to allow for simultaneous computations of different states alleviating the use of globally defined chaos polynomials.

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MS116

Uncertainty Quantification for a Biomedical Blood Pump Application

The Finite Element Method (FEM) has been extensively employed for the development of mechanical devices. A huge amount of devices are today realized owing to numerical simulation by finite elements. This also holds for our studied application, the ventricular assist device, which is one of the most common therapeutic instruments for the cardiac insufficiency. The functional reliability of biomedical devices remains one of the main concerns for the utilization in different clinical areas. This especially holds for our blood pump application. Computational Fluid Dynamics could help to simulate the basic functionality of the device. However, there are still uncontrollable aspects, which cannot be determined by classical numerical methods, due to noisy data, or the lack of knowledge about physical phenomena. Here, Uncertainty Quantification (UQ) fills the gap. In this work, we model a blood pump device with consideration of the uncertainty. We study three uncertain parameters (kinematic viscosity, angular velocity and inflow amplitude), which are the most important parametric variations in the model, in order to analyze the influence on the numerical solution. Concerning to the rotation of the blood pump, we employ the Sliding Mesh method, which gives good results for symmetric rotating systems. We also apply the Variational Multiscale method to stabilize the incompressible Navier-Stokes equations. In our talk, we will present our latest research results.

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MS117

Title Not Available

Abstract not available.

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MS117

Quasi-Monte Carlo and FFT Sampling for Elliptic PDEs with Lognormal Random Coefficients

We generalise and study the convergence analysis of a method which was computationally presented by the authors in J. Comp. Phys. in 2011, where a quasi-Monte Carlo method combined with a circulant embedding/FFT method was used to sample from a lognormal random field. The method allows to sample form very rough random fields without the need to truncate a KL series expansion.

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MS117

Gradient-Free Active Subspace Construction Via Adaptive Morris Indices

In this presentation, we present a gradient-free algorithm for constructing active subspaces for physical and biological applications having high-dimensional input spaces. The objective of this approach is two-fold: determine low-dimensional active input spaces for high-dimensional problems and construct surrogate models based on these reduced spaces. Whereas there exist a variety of algorithms to construct low-dimensional subspaces when gradients are available, a number of production codes do not provide gradient or adjoint capabilities. To accommodate these applications, we consider a gradient-free approach in which adaptive Morris indices are used to construct the reduced input space. In this approach, steps are adapted to dominant directions in the parameter space to improve the accuracy and efficiency of algorithms. Attributes of the method are demonstrated for examples arising in aerodynamics and nuclear power plant design.

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MS117

Cross Validation for Function Approximation: Quantitative Guarantees and Error Estimates

Using tools from compressive sensing and matrix concentration, we provide quantitative guarantees for the accuracy of leave-p-out cross validation towards model selection and error estimation in function interpolation and approximation problems. The guarantees are 'with high probability' with respect to the stochastic sampling points.

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MS118

A Space-time Fractional Optimal Control Problem: Analysis and Discretization

We study a linear-quadratic optimal control problem involving a parabolic equation with fractional diffusion and Caputo fractional time derivative of orders $s \in (0,1)$ and $\gamma \in (0,1]$, respectively. The spatial fractional diffusion is realized as the Dirichlet-to-Neumann map for a nonuniformly elliptic operator. Thus, we consider an equivalent formulation with a quasi-stationary elliptic problem with a dynamic boundary condition as state equation. The rapid decay of the solution to this problem suggests a truncation that is suitable for numerical approximation. We consider a fully-discrete scheme: piecewise constant functions for the control and, for the state, first-degree tensor product finite elements in space and a finite difference discretization in time. For $s \in (0,1)$ and $\gamma < 1$ we show convergence of this scheme. Moreover, under additional regularity, we derive a priori error estimates for the case $s \in (0,1)$ and $\gamma = 1$.

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MS118

Length Scale and Manufacturability of Topology Optimized Designs

Topology optimization as a design methodology is widely accepted in the industry. The designs are often considered conceptual due to loosely defined topologies and the need of post processing. Amendments can affect the performance and in many cases can completely destroy the optimality of the solution. Therefore, the goal of this work is to present recent advancements in obtaining manufacturable designs with clearly defined minimum length scale and performances robust with respect to production uncertainties.

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MS118

Managing Uncertainty in PDE-Constrained Optimization Using Risk Measures

We consider PDE-constrained optimization problems under uncertainty. In order to manage the risk due to the implicit dependence of the state with respect to the random variables, we make use of coherent risk measures, which yield risk-averse optimal solutions. First-order optimality conditions for the resulting non-smooth problems are derived via an epi-regularization technique that is directly linked to a numerical method. The results are illustrated by several numerical examples.

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MS118

Constrained Optimization with Low-Rank Tensors and Applications to Problems with Pdes under Uncertainty

We present Newton-type methods for inequality constrained nonlinear optimization using low-rank tensors and apply them to variational inequalities with several uncertain parameters and to optimal control problems with PDEs under uncertainty. The developed methods are tailored to the usage of low-rank tensor arithmetics, which only offer a limited set of operations and require truncation (rounding) in between. We show that they can solve huge-scale optimization problems with trillions of unknowns to a good accuracy.

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MS119

The Discrete Empirical Interpolation Method for the Steady-State Navier-Stokes Equations

We examine the discrete empirical interpolation method (DEIM) for solving the discrete steady-state Navier-Stokes equations where the viscosity is a random field. We explore the impact of number of interpolation points on the accuracy of DEIM solutions and show that essentially full accuracy is obtained with fewer than 100 points, a number typically much smaller then the dimension of the reduced

model. In addition, we develop preconditioning operators for solving the algebraic equations that arise from DEIM and demonstrate that preconditioned solvers are effective when the size of the parameter space is large.

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MS119

Reduced-Order Modeling Of Hidden Dynamics

The objective of this paper is to investigate how noisy and incomplete observations can be integrated in the process of building a reduced-order model. This problematic arises in many scientific domains where there exists a need for accurate low-order descriptions of highly-complex phenomena, which can not be directly and/or deterministically observed. Within this context, the paper proposes a probabilistic framework for the construction of "POD-Galerkin" reduced-order models. Assuming a hidden Markov chain, the inference integrates the uncertainty of the hidden states relying on their posterior distribution. Simulations show the benefits obtained by exploiting the proposed framework.

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MS119

A Triple Model Reduction for Data-Driven Large-Scale Inverse Problems in High Dimensional Parameter Spaces

We present an approach to address the challenge of data-driven large-scale inverse problems in high dimensional parameter spaces. The idea is to combine a goal-oriented model reduction approach for state, data-informed reduction for parameter, and randomized misfit approach for data reduction. The method is designed to mitigate the bottle neck of large-scale PDE solve, of high dimensional parameter space exploration, and of ever-increasing volume of data. Various numerical results are conducted to support the proposed approach.

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MS119

POD-Galerkin Modeling with Adaptive Finite Elements for Stochastic Sampling

We study surrogate models for time-dependent PDEs with uncertain data. To include spatial adaptivity, we generalize proper orthogonal decomposition (POD) based reduced-order modeling to snapshots from different finite element spaces. We analyze how this generalization effects sampling based uncertainty quantification and comment on the implementation for nested spatial grids. A numerical test case involving a 2d Burgers equation with uncertain initial data confirms the theoretical findings.

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MS120

Local Optimal Rotation for Min-mode Calculation in Computing Transition State

Abstract not available.

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MS120

A Convex Splitting Scheme for the Saddle Point Search in Phase Filed Model

The convex splitting method has been very successful in maintaining unconditional energy stability in evolving the steepest descent dynamics for phase field model, which is of particularly use to search local minima of energy landscape since large time step is allowed. In this work, we generalize this idea to the challenging problem of searching transition states, i.e., index-1 saddle points. By using the Iterative Minimization Formulation, the saddle point problem is progressively solved by a series of minimization problems. We show how the convex splitting method still plays a key role in searching saddle point by numerical results of Allen-Cahn equation, Cahn-Hilliard equation and the McKean Vlasov equation.

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MS120

The String Method for the Study of Rare Events

The string method is an effective numerical tool for computing minimum energy paths between two meta-statble states. It evolves a string in the path space by the steepest descent dynamics. In this talk, we show how the string method can be used to compute saddle points (transition states) for a given minimum of the potential or free energy. These saddle points act as bottlenecks for barrier-crossing events. Application to the wetting transition on patterned surfaces will be presented.

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MS120

Quantifying Transition Dynamics of Nanoscale

Complex Fluid via Mesoscopic Modeling

Abstract not available.

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MS121

Learning to Optimize with Confidence

Abstract not available.

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MS121

Stratified Bayesian Optimization

Abstract not available.

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MS121

Empirical Orthogonal Function Calibration with Simulator Uncertainty

Abstract not available.

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MS121

Variational Bayesian Inference Using Basis Adaptation in Homogeneous Chaos Surrogates

The problem of subsurface characterization in reservoir modeling under uncertainty undergoes several computational challenges, two of them typically being the high dimensionality of the random fields involved in the description of the rock properties and the expensive reservoir models involved in uncertainty propagation. We present a novel dimension reduction method that is applicable when the true models are substituted by Wiener Polynomial Chaos surrogates. The method involves adapting the basis of the underlying Gaussian Hilbert space such that the probability measure of the original Chaos expansion is concentrated in a lower dimensional space of the new adapted expansion. The attractiveness of our methodology is highlighted when applied as a dimensionality reduction technique within a Variational Bayesian inference (VI) framework in order to efficiently solve inverse problems.

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MS122

Marginal Then Conditional Sampling for Hierarchical Models

Independent sampling in the linear-Gaussian inverse problem may be performed for less computational cost than regularized inversion, when selection of the regularizing parameter is considered. We demonstrate a sequence of increasingly efficient sampling algorithms: block Gibbs, one-block, and the 'marginal-then-conditional' sampler with a fancy method for evaluating the ratio of determinants required for MCMC. This last method scales well with problem and data size, allowing inference over function space models with no approximation (!).

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MS122

Sampling Gaussian Distributions in High Dimensional Statistical Inference

Direct sampling of a multivariate Gaussian distribution is traditionally performed using a Cholesky factorization of the covariance/precision matrix. In this talk, we recall existing techniques to avoid the Cholesky factorization and describe a new method that uses the reversible jump MCMC framework to derive a convergent Gaussian sampler involving approximate resolution of a linear system. We also present an unsupervised adaptive scaling of the proposed sampler to minimize computation cost per effective sample.

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MS122

Fast Sampling for Inverse Equilibrium Problems

We present efficient numerical methods for posterior exploration by Metropolized approximate Gibbs sampling of $\mathbf{A}^T\mathbf{C}\mathbf{A}$ systems that occur throughout science and engineering. The presented methods cover efficient simulation of the system class as well as the numerically cheap evaluation of low rank updates and approximate conditional sampling. In numerical tests, sampling from this nonlinear inverse problem incurs little more cost than the best

samplers for linear-Gaussian inverse problems.

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MS122

Fitting Lateral Transfer: MCMC for a Phylogenetic Likelihood Obtained from a Massive Linear ODE System

We give a Bayesian sample-based inference procedure for reconstructing the phylogenies of taxa from evolutionary traits when diversification is not strictly tree-like, but may include lateral transfer. The likelihood for a tree with L leaves is determined from the solution of a sequence of sparse linear ODEs of dimension up to $2^L - 1$. We propose an exact approach exploiting symmetries in Green's functions for small L and MCMC methods for larger values of L.

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MS123

Nonlinear Statistical Analysis Based on Imprecise Data

Abstract not available.

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MS123

Modelling with Random Sets in Engineering

When assessing the response of a mechanical structure, loads, material and geometric parameters enter as inputs. As a rule, knowledge about these parameters is incomplete. The theory of random sets permits to combine interval methods and stochastics for quantifying the uncertainties. The talk addresses modelling with random sets combined with random fields, simulating the uncertain structural response, sensitivity analysis and selected applications in elastostatics and structural dynamics.

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MS123

Dealing with Limited and Scarse Information in Complex Systems and Critical Infrastructures

Critical infrastructures are ensembles of assets, organizations and complex network layers (e.g. power network, information network, etc.) which reliability is of major concern for the people safety and well-being. In some cases, systems data might result unavailable or parts of information lost or modified when transferred or processed. In order to deal with uncertainty arising from scarce or inconsistent data, classical probabilistic approaches are sometime used, although requiring assumptions to model imprecision, sometime hardly justifiable. Unwarranted hypothesis can alter the apparent level of uncertainty and system reliability. Imprecise probabilistic methods offer a solid grounding for the rational treatment of uncertainty due to scarce and imprecise data, powerful frameworks which can be coupled to traditional methods to better understand the true quality of the information and effective system reliability.

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MS123

Nonparametric Bayesian Estimation of System Reliability with Imprecise Prior Information on Component Lifetimes

Estimation of reliability functions for complex systems is usually based on component test data. As data is often scarce, expert information must be included, which is often also vague and imprecise. Such uncertain but influential expert information can be combined with test data using a flexible imprecise Bayesian nonparametric approach producing sets of posterior predictive system reliability functions that reflect uncertainty in expert information, the amount of data, and provides prior-data conflict sensitivity.

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MS124

Approximation of Probability Density Functions by the Multilevel Monte Carlo Maximum Entropy Method

We develop a complete convergence theory for the Maximum Entropy method based on moment matching for a sequence of approximate statistical moments estimated by the Multilevel Monte Carlo method. Under appropriate regularity assumptions on the target probability density function, the proposed method is superior to the Maximum Entropy method with moments estimated by the Monte Carlo method. New theoretical results are illustrated in numerical examples. We compare our approach with an alternative MLMC-based method by M. Giles, T. Nagapetyan and K. Ritter (2015) and comment on the benefits and drawbacks.

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MS124

Efficient Coupling of Multi-Level Monte Carlo Method with Multigrid

We study the benefits of combining multigrid with multi-level Monte Carlo (MLMC). We consider groundwater flow using an elliptic PDE with lognormal random hydraulic conductivity fields. The solution is based on a finite volume discretization that is solved with a cell-centered multigrid (CCMG). We show through numerical experiments how we can achieve greater computational savings by using same set of MLMC levels in the multigrid solvers.

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MS124

MLMC with Control Variate for Lognormal Diffusion

We consider the stochastic Darcy problem with log-normally distributed permeability field and propose a novel MLMC approach with control variate variance reduction technique on each level. We model the log-permeability as a stationary Gaussian random field with Matérn covariance. The control variate is obtained by solving an auxiliary problem with smoothed permeability field and its expectation is effectively computed with a Stochastic Collocation method on the finest level in which the control variate is applied.

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MS124

A Multiscale Model and Variance Reduction Method for Wave Propagation in Heterogeneous Materials

We present a model and variance reduction method for computing statistical outputs of stochastic wave propagation problems through heterogeneous materials. We combine the multiscale continuous Galerkin (MSCG) discretization and the reduced basis method for the Helmholtz equation with a multilevel variance reduction strategy, exploiting the statistical correlation among the MSCG and reduced basis approximations to accelerate the convergence of Monte Carlo simulations. We analyze the effect of manufacturing errors on waveguiding through photonic crystal structures.

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MS125

Optimal Experimental Design for ODE Models

Recovering parameters from ODE models can be inherently hard. Due to dimensionally, complexity, and sensitivity of the model states and parameters, robust parameter estimation methods are needed. We will present robust parameter estimation approaches that will guide optimal experimental design methods towards accurate recovery of model parameters.

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MS125

A Layered Multiple Importance Sampling Scheme for Focused Optimal Bayesian Experimental Design

The optimal selection of experimental conditions is essential to maximizing the value of data for inference and prediction, particularly in situations where experiments are costly. We propose an information theoretic framework for focused experimental design with simulation-based models, with the goal of maximizing information gain in targeted subsets of model parameters. A novel layered multiple importance sampling technique is used to efficiently evaluate the expected information gain to make optimization feasible for computationally intensive and high-dimensional problems.

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MS125

Variance Reduction Methods for Efficient Bayesian Experimental Design

We propose a framework where a lower bound of the expected information gain is used as an alternative design criterion in order to compute Bayesian optimal experimental designs. In addition to alleviating the computational burden, this also addresses issues concerning estimation bias. The validity of our approach is demonstrated in parameter inference problems concerning flow and transport in porous media where and Polynomial Chaos approximations of the forward models are constructed that further accelerate the objective function evaluations.

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MS125

Efficient Computation of Bayesian Optimal Designs

In Bayesian inference, fast and reliable estimation and maximization of the expected information gain with respect to alternative setups is crucial to provide a valuable orientation toward the planning of future experiments. This talk focuses on efficient methods for obtaining approximations to the posterior distribution in Bayesian design problems. Examples related to inverse heat conduction problems will illustrate the effectiveness of such approaches in order to recommend to the practitioner the best allocation of resources.

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MS126

Stochastic Collocation for Differential Algebraic Equations Arising from Gas Network Simulation

We use the method of stochastic collocation to quantify the uncertainties arising from the stochastic parameters of the differential algebraic equations. Due to the method's non-intrusiveness we can apply a commercial gas network simulator to compute a stationary solution for a given parameter set. Since in DAEs only derivatives of a part of variables are incorporated, the solution is typically non-differentiable. We present a method to overcome the existing kinks and show some numerical convergence results.

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MS126

Parametric Uncertainty in Macroscopic Traffic Flow Models Calibration from Gps Data

Facing the problem of macroscopic traffic flow models calibration with Floating Car Data from GPS devices, we propose to introduce the dependence from stochastic parameters in the mean velocity closure equation and the initial density profile. We use a semi-intrusive deterministic approach to quantify uncertainty propagation in traffic density evolution and travel-times estimation. Numerical results are presented. The approach is then validated on processed real data on a stretch of highway in South-East France.

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MS126

On a Data Assimilation Method Coupling Kalman Filtering, MCRE Concept, and PGD Model Reduction for Real-Time Updating of Structural Mechanics Models

This work introduces a new strategy for real-time parameter identification or updating in structural mechanics models, defined as dynamical systems. The main idea is to use the Unscented Kalman filtering, which is a Bayesian data assimilation method, in conjunction with an energetic method for inverse problems, the modified Constitutive Relation Error. A PGD model reduction is also introduced to perform real-time computations. The proposed approach is illustrated, and compared to classical approaches, on several applications.

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MS126

Sequential Design of Computer Experiments for the Solution of Bayesian Inverse Problems

We present an adaptive sampling method for the solution of Bayesian parameter inference problems. The model function is assumed to be computationally expensive, so the goal is to approximate the posterior with as few function evaluations as possible. To this end, the a priori unknown model function is described by a process emulator, and in each iteration, a new point is selected such that the estimated impact on the accuracy of the posterior distribution is maximized.

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MS127

Separating Discretization Error and Parametric Uncertainty in Goal-Oriented Error Estimation for

Pdes with Uncertainty

We revisit our earlier work on goal-oriented error estimation for partial differential equations with uncertain data, where error estimates were decomposed into contributions from physical discretization and the approximation in parameter space. We provide a detailed examination of the error estimation and decomposition process for a nonlinear model problem; effectivity indices, error indicators, and adaptive strategies are discussed. Finally, we present the application of the framework to Bayesian model selection for turbulence modeling.

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MS127

Error Estimation and Adaptivity for PGD Reduced Models

A prominent model reduction technique based on low-rank canonical format, and referred as Proper Generalized Decomposition (PGD), was recently introduced for the numerical solution of high-dimensional problems. In the PGD framework, an a posteriori error estimate based on dual analysis was proposed, enabling to assess contributions of various error sources. In the present work, we address new advances in this verification method, considering parameters of all kinds, and nonlinear problems.

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MS127

Adaptive Stochastic Galerkin Fem with Hierarchical Tensor Representation

PDE with stochastic data usually lead to very high-dimensional algebraic problems which easily become unfeasible for numerical computations because of the coupling structure of the discretised stochastic operator. Recently, an adaptive stochastic Galerkin FEM based on a residual a posteriori error estimator was presented and the convergence of the adaptive algorithm was shown. While this approach leads to a drastic reduction of the complexity of the problem due to the iterative discovery of the sparsity of the solution, the problem size and structure is still rather limited. To allow for larger and more general problems, we exploit the tensor structure of the parametric problem by representing operator and solution iterates in the tensor train (TT) format. The (successive) compression carried out with these representations can be seen as a generalisation of some other model reduction techniques, e.g. the reduced basis method. We show that this approach facilitates the efficient computation of different error indicators related to the computational mesh, the active polynomial chaos index set, and the TT rank. In particular, the curse of dimension is avoided.

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MS127

A Posteriori Error Estimates for Navier-Stokes Equations with Small Uncertainties

We perform *a posteriori* error analysis for the steady-state incompressible Navier-Stokes equations defined on random domains. We use the so-called domain mapping method that yields PDEs on a fixed domain with random coefficients. With a perturbation approach, we expand then the exact solution with respect to a parameter ε that controls the amount of uncertainty. We derive error estimates accounting the two sources of error and give numerical examples to illustrate the theoretical results.

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MS128

History Matching with Structural Reliability Methods

History matching is an inverse problem methodology that identifies subsets in the input space of an expensive computer model, such that the output is likely to have a good fit with observed data. Its efficiency depends on the evaluation of an implausibility function and on the iterative sampling on the reduced input space. We present a sampling strategy based on Subset Simulation, an efficient technique developed and used to solve structural reliability problems.

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MS128

Efficient Inverse Problems with Gaussian Process Surrogates Via Entropy Search

Scientists often express models through computer simulators, and Gaussian process emulation of these simulators provides an effective way to reduce computation when interrogating such a model. Meanwhile, Bayesian optimisation has gained popularity, where a Gaussian process emulator is used to provide information-theoretic guidance for finding extrema of functions. Here, we combine these ideas, proposing a method for solving inverse problems guided by entropic search. The method is demonstrated on a simple model of climate.

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MS128

Bayesian Inference for Linear Parabolic PDEs with Noisy Boundary Conditions

Many real problems require inferring the coefficients of linear parabolic PDEs under the assumption that noisy measurements are available in the interior of a domain of interest and for the unknown boundary conditions. This talk will focus on solving the inverse problem by using hierarchical Bayesian techniques based on the marginalization of the contribution of the boundary parameters. Inverse heat conduction problems for simulated and real experiments under different setups will illustrate the proposed approach.

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MS128

Iterative History Matching for Computationally Intensive Inverse Problems

Iterative History Matching using Bayes Linear statistics has been shown to be a very successful methodology for solving inverse problems for computationally intensive models. We will discuss recent advances in this area including nested emulator approximations and fast output scans for efficient input space reduction. We will describe how history matching provides a natural framework for designing future experiments tailored to resolving specific uncertainties uncovered in the inverse calculation, with a systems biology application.

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MS129

Regression-Based Adaptive Sparse Polynomial Dimensional Decomposition for Sensitivity Analysis in Fluids Simulation

Polynomial dimensional decomposition (PDD) is employed in this work for global sensitivity analysis and uncertainty quantification of stochastic systems subject to a large number of random input variables. Due to the intimate structure between PDD and Analysis-of-Variance, PDD is able to provide simpler and more direct evaluation of the Sobol sensitivity indices, when compared to polynomial chaos (PC). This work proposes a variance-based adaptive strategy aiming to build a cheap meta-model by sparse-PDD with PDD coefficients computed by regression. The size of the final sparse-PDD representation is much smaller than the full PDD, since only significant terms are eventually retained.

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MS129

Effective Improvement of Aerodynamic Performance over a Parameter Interval

Accounting for uncertainties is now a requirement in aircraft design. However, classical robust optimization methods, based on statistical criteria (mean, variance, etc), cannot guarantee an effective improvement of the aerodynamic performance over the whole interval of variation of uncertain parameters. We propose here an extension of the steepest-descent method, that allows to define a descent direction common to a large set of functionals parameterized by the uncertain parameters. Illustrations will include uncertainties arising from flow conditions and time-dependency.

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MS129

Adaptive Surrogate Modeling Strategies for Efficient Bayesian Inference

Polynomial surrogates have recently been proposed to reduce the computational cost of Bayesian inference. In regions of low posterior probability, the construction of accurate surrogates is however wasteful. We propose a novel adaptive construction of the surrogate where additional model evaluations in high posterior regions are taken into account to progressively improve the approximation. The method is tested on several academic examples to illustrate its effectiveness.

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MS129

Time-Optimal Path Planning in Uncertain Flow Field Using Ensemble Method

We focus on time-optimal path planning in uncertain flows. Uncertainty is represented in terms of a finite-size ensemble, and for each ensemble member a deterministic time-optimal path is predicted. This enables us to perform a statistical analysis of travel times, and consequently develop a path planning approach that accounts for these statistics. The performance of the ensemble representation is analyzed, and the simulations are used to develop insight into extensions dealing with general circulation forecasts.

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MS130

Bayesian Inference and Model Selection in Molecular Dynamics Simulations

Abstract not available.

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MS130

Path-Space Information Criteria and Uq Bounds for the Long-Time Behavior of Extended Stochastic Systems

Abstract not available.

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MS130

No Equations, No Variables: Data, and the Computational Modeling of Complex Systems

Abstract not available.

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MS130

Coarse-Graining of Stochastic Dynamics

Abstract not available.

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MS131

Successive Approximation of Nonlinear Confidence Regions (SANCR)

In parameter estimation problems an important issue is the approximation of confidence regions. These can be nonlinear and, in case of bad conditioning of the estimation problem, strongly elongated. Therefore, their approximation can be computationally highly expensive, especially for differential equations. To combine high accuracy and low computational costs, we have developed a method that uses only successive linearizations in the vicinity of an estimator. We show the potential of this method by numerical examples.

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MS131

Uncertainty Quantification for Crosswind Stability of Vehicles

The objective of uncertainty quantification for crosswind stability is the computation of failure probabilities for a non-stationary realistic gust model with random amplitude and duration. In addition, the strongly nonlinear aerodynamic coefficients, which highly depend on the vehicle shape as well as the relative wind angle, are modeled as random variables. Failure probabilities can be obtained either conditioned on a certain mean wind speed and direction or a certain physical scenario. They are based on limit states for the safe operation of the vehicle.

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MS131

Towards Meshless Uncertainty Quantification in Medical Imaging on GPUs

In cancer diagnosis, radiological imaging is one of the only non-invasive ways to decide whether tissue is subject to cancer or not. However, radiological images are subject to high variabilities due to imaging errors, patient movement, etc. In the recent years, the extraction of imaging biomarkers (e.g. features or meta-data) from radiological images is a growing research topic. Imaging biomarkers shall be reliable diagnosis indicators for cancer. However, these biomarkers are assumed to be subject to a high variability based on the underlying image variability. The purpose of our ongoing research endeavour is to find ways to overcome this variability and thereby to make the overall biomarker extraction pipeline more reliable. Here, one crucial part is the appropriate quantification of stochastic moments of biomarkers and images. In the recent years, we have introduced the meshless kernel-based stochastic collocation using radial basis functions. This non-intrusive UQ method is designed to solve large-scale problems in a high-order convergent and scaling fashion. We are about to integrate our method into the appropriate imaging tool pipeline of radiologists. Moreover, we aim at performing our full analysis on graphics processing units, to be able to integrate the software in imaging devices, in the long run. In our presentation, we will give the latest results on the

described developments.

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MS132

Uncertainty Propagation Estimates with Semidefinite Optimization

We show how tight estimates on the support of the push-forward of a probability measure through a non-linear semi-algebraic mapping can be obtained by moment-sum-of-squares hierarchies and convex semidefinite programming.

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MS132

Global Sensitivity Analysis for the Boundary Control of An Open Channel

We consider the boundary control problem of an open-water channel, whose boundary conditions are defined by the position of a downstream overflow gate and an upperstream underflow gate. Water depth and velocity are described by Shallow-Water equations. As physical parameters are unknown, a stabilizing boundary control is computed for their "nominal" values, and then a sensitivity analysis is performed to measure the impact of uncertainty in parameters on a given to-be-controlled output.

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MS132

Worst-Case Robustness Analysis and Synthesis in Control

We give an overview over key ideas how to handle parametric and non-parametric uncertainties in control. A main emphasis will be laid on robust stability and performance analysis techniques that are based on dissipation arguments and dedicated tools from robust semi-definite programming. We highlight the difficulties that arise in designing robust controllers and address paths how they can be overcome. If time permits we point out relations to stochastic uncertainty descriptions.

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MS132

Uncertainty Randomization in Control Systems

It is well-known that uncertainty leads to a significant performance degradation of control systems. At the beginning of this lecture, we illustrate this fact using a simple example and discuss two alternative approaches: robust and stochastic. Subsequently, we provide a perspective of randomized techniques to handle uncertain stochastic systems. In particular, we introduce the notion of sample complexity, demonstrate its key role in feedback systems, and study related probabilistic bounds. Regarding control design, we formulate a robust optimization approach for both convex and nonconvex problems. Finally, connections with statistical learning theory will be outlined.

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MS133

Renewable Energy Integration in the Central Western European System

This paper presents a detailed model of the current market coupling mechanism in the Central Western European system. Market coupling is compared against deterministic and stochastic unit commitment under current renewable energy integration levels. Efficiency losses of the market coupling model with respect to deterministic unit commitment are estimated to range between 2.8%-6.0%. Efficiency gains of stochastic with respect to deterministic unit commitment are estimated at 0.9%.

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MS133

Multi-Timescale Stochastic Power Systems Operation with High Wind Energy Penetration

We present a novel set of stochastic unit commitment and economic dispatch models that consider stochastic loads and variable generation at four distinct but interconnected operational timescales. Comparative case studies with deterministic approaches are conducted in low wind and high wind penetration scenarios to highlight the advantages of the proposed methodology. The effectiveness of the proposed method is evaluated with sensitivity tests using both economic and reliability metrics to provide a broader view of its impact.

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MS133

Introducing Uncertainty to Transmission Expansion Planning Models A North Sea Case Study

Grid investments are sunk costs with a long lifetime, and the market fundamentals for cost recovery is experiencing increased share intermittent power production. To cope with the changing market environments and alternative flexibility options it is of great importance to improve TEP models to account for both uncertainty and enhanced modelling of market operation. The progressive hedging algorithm is applied to a MILP for transmission expansion planning, as a first stage towards a stochastic model.

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MS133

Adaptive Sparse Quadrature for Stochastic Optimization

Monte Carlo (MC) techniques are commonly used to estimate statistics, e.g. expectations, employed in stochastic optimization models. While generally robust, the MC approach exhibits poor convergence properties. Here we consider an alternate approach, modeling uncertain parameters as random variables and employing Polynomial Chaos expansions (PCEs) to efficiently propagate uncertainties from model inputs to outputs. These PCEs are constructed adaptively via sparse quadrature. The performance of this approach is compared with results based on classical formulations.

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MS134

Non-Degenerate Particle Filters in High-Dimensional Systems

The general solution of the data assimilation problem can be found using Bayes' theorem. In practice, however, it is virtually impossible to evolve probability density functions in time and update them with the likelihood of observations. Particle filters rely in samples to estimate the posterior probability density function. Traditional particle filters, however, can suffer from degeneracy when the system size (actually number of independent observations) is not small. In this work we present a formulation that a) explores regions of high probability making use of future observations and b) does not become degenerate by selecting updating positions of the particles considering the statistical characteristics of the whole ensemble (and not just the individual particle being updated).

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MS134

Hybrid Particle - Ensemble Kalman Filter for Lagrangian Data Assimilation

Lagrangian data such as those collected by gliders or floats in the ocean are highly nonlinear and their assimilation into high-dimensional models of the velocity field is a challenging task. We present a hybrid filter that applies the EnKF update to velocity variables and the PF update to drifter variables. We present some results from this hybrid filter applied to high-dimensional quasi-geostrophic ocean model and compare those to results from standard ensemble Kalman filter and ensemble runs without assimilation.

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MS134

Accuracy and Stability of Nonlinear Filters

Abstract not available.

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MS134

Sequential Implicit Sampling Methods for Bayesian Inverse Problems

The solution to the inverse problems, under the Bayesian framework, is given by a posterior probability density. For large scale problems, sampling the posterior can be an extremely challenging task. Markov Chain Monte Carlo (MCMC) provides a general way for sampling but it can be computationally expensive. Gaussian type methods, such as Ensemble Kalman Filter (EnKF), make Gaussian assumptions even for the possible non-Gaussian posterior, which may lead to inaccuracy. In this talk, the implicit sampling method and the newly proposed sequential implicit sampling methods are investigated for the inverse problem involving time-dependent partial differential equations (PDEs). The sequential implicit sampling method combines the idea of the EnKF and implicit sampling and it is particularly suitable for time-dependent problems. Moreover, the new method is capable of reducing the computational cost in the optimization, which is a necessary and most expensive step in the implicit sampling method. The sequential implicit sampling method has been tested on a seismic wave inversion. The numerical experiments shows its efficiency by comparing with the MCMC and some Gaussian approximation methods.

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MS135

Spectral Analysis of Stochastic Networks

Stochastic networks with pairwise transition rates of the form $L_{ij} = \exp(-U_{ij}/T)$ where T is a small parameter (the absolute temperature in the physical context) arise in modeling of rare events in complex physical systems. I will introduce methods for finding the spectral decomposition of the generator matrices of such networks in the limit $T \to 0$, finite temperature continuation techniques, and an application to the problem of the Lennard-Jones-75 cluster rearrangement.

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MS135

Vortices in the Stochastic Parabolic Ginzburg-Landau Equation

We consider the variant of a stochastic parabolic Ginzburg-Landau equation that allows for the formation of point defects of the solution. We show that the family of the Jacobians associated to the solution is tight on a suitable space of measures. Its limit points are concentrated on finite sums of delta measures with integer weights. This provides the definition of the stochastic Ginzburg-Landau vortices. We shall also discuss the possibility to study, within our framework, the noise-induced nucleation of vortices.

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MS135

Competition Between Energy and Entropy in the Stochastic Allen-Cahn Equation

We will comment on the competition between energy and entropy in stochastically perturbed systems. We focus on the example of the stochastic Allen-Cahn equation, for which we have analyzed the invariant measure in joint work with Felix Otto and Hendrik Weber. While for small noise strength a transition between the favored states is energetically penalized, a large system size means that there are many places at which such a rare event may take place. Our first result quantifies this competition.

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MS135

Packing and Unpacking

Abstract not available.

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MS136

VPS: Voronoi Piecewise Surrogates for High-Dimensional Data

We introduce VPS: a new method to construct credible global high-dimensional surrogates, using an implicit Voronoi tessellation around black-box function evaluations. The neighborhood network between cells (approximate Delaunay graph) enables each cell to build its own local piece of the global surrogate taking advantage of intrusively generated information, e.g., derivatives. Due to its piecewise nature, VPS accurately handles smooth functions with high curvature as well as functions with discontinuities, and can adopt a parallel implementation.

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MS136

A Hybrid Approach to Tackle Resiliency in Extreme Scale Computations Using a Domain Decomposition Solver for Uncertain Elliptic Pdes

One challenging aspect of extreme scale computing concerns combining UQ methods with resilient PDE solvers. We present a resilient polynomial chaos solver for uncertain elliptic PDEs. The solver involves domain decomposition for tackling extreme scale problems, robust regression techniques to provide resilience, and spectral methods for the UQ. Our hybrid UQ approach mixes a resilient non-intrusive approximation of stochastic Dirichlet-to-Dirichlet maps and a Galerkin projection to determine the solution at the subdomain interfaces.

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MS136

A Soft and Hard Faults Resilient Solver for 2D Uncertain Elliptic PDEs via Fault-tolerant MPI Server-client-based Implementation

We discuss an approach to solve 2D elliptic PDEs with uncertain coefficients that incorporates resiliency to soft and hard faults. Resiliency to soft faults is obtained at the algorithm level by recasting the PDE as a sampling problem followed by a resilient manipulation of the data to obtain a new solution. Resiliency to hard faults is achieved at the implementation level by leveraging a fault-tolerant MPI implementation (ULFM-MPI) within a task-based server-client model.

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MS137

Dimension Reduction for UQ in Satellite Retrieval Methods

Many satellite instruments observe reflected or transmitted solar or even stellar radiation. Retrieving information of vertical gas density profiles of atmospheric constituents, such as ozone, is an ill-posed inverse problem and a priori information must be incorporated to solve it. Using sampling-based estimation and uncertainty quantification with dimension reduction, we can solve the problem directly in a suitable low dimensional subspace of the full solution. In this presentation, we discuss dimension and model reduction for selected satellite instruments and retrieval algorithms. We utilize likelihood-informed dimension reduction with adaptive MCMC to retrieve profile information matching the degrees of freedom in the observations.

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MS137

Efficient Scalable Variational Bayesian Approximation Methods for Inverse Problems

When using hierarchical prior models for Bayesian inference for inverse problems, the expression of the joint posterior law is complex and analytical computations often impossible. MCMC method are then common tools but unfortunately they are not scalable. Variational Bayesian Approximation methods are alternatives which can efficiently be used. In this work we show a few implementations of these methods for Image Reconstruction in Computed Tomography.

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MS137

Optimization-Based Samplers using the Framework of Transport Maps

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, for example randomize-then-optimize (RTO), repeatedly solve optimization problems to obtain proposal samples. We analyze RTO using a new interpretation that describes each optimization as a projection and as the action of an approximate transport map. From this analysis, several new variants of RTO — adaptive RTO, mixtures of RTO proposals, and transformed random walks — follow naturally.

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MS137

Quantifying Model Error in Bayesian Parameter Estimation

In complex Bayesian hierarchical models, the posterior distribution of interest is often replaced by a computationally efficient approximation to make Markov chain Monte Carlo algorithms feasible. In this work, we propose statistical methodology that utilizes high performance computing and allows one to quantify the model error, defined as the discrepancy between the target and approximate posterior distributions. This provides a structure to analyze model approximations with regard to the impact on inference and computational efficiency.

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MS138

Probabilistic Formulations of Elementary Algorithms in Linear Algebra and Optimization

Broad practical success of error estimation in numerical methods hinges on computational cost. Ideally, adding a well-calibrated error estimate to a classic numerical point estimate should have no, or only very limited computational overhead. This talk will start with the observation that several basic numerical methods can directly be interpreted as maximum a-posteriori estimates under certain families of Gaussian priors (the focus will be on algorithms for linear algebra and optimization). By itself, however, this connection does not yield a unique calibration for the posterior's width. I will point out technical challenges and opportunities for such calibration at runtime, which give varying degrees of error calibration in return for a correspondingly varying amount of computational effort.

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MS138

Bayesian Inference for Lambda-coalescents: Failures and Fixes

The class of Lambda-coalescents arise as models of genetic ancestry of populations with reproductive skew. In this talk I show that naively sampling DNA from such a population and applying Bayesian inference with a Lambda-coalescent prior leads to inconsistent inference with high sensitivity to the observation and to hyperparameters. These issues can be resolved by temporally structured sampling and carefully chosen inference algorithms, which are able to yield provably consistent and robust inference.

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MS138

Opportunity for Uncertainty in Cardiac Modelling

Biophysical computational models of individual patients hearts represent a novel framework for understanding the mechanisms behind disease, selecting patients and optimising treatments. Personalising computational models from noisy and sparse clinical data increasingly represents the limiting step in simulation workflows while propagation of that uncertainty through to model predictions is routinely absent. This presentation describes the problem and outlines our progress in engaging uncertainty quantification in the development and simulation of cardiac models.

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MS138

Brittleness and Robustness of Bayesian Inference

It is natural to investigate the accuracy of Bayesian procedures from several perspectives: e.g., frequentist questions of well-specification and consistency, or numerical analysis questions of stability and well-posedness with respect to perturbations of the prior, the likelihood, or the data. This talk will outline positive and negative results (both classical ones from the literature and new ones due to the authors and others) on the accuracy of Bayesian inference in these senses.

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MS139

A Gaussian Process Trust Region Method for Stochastic Constrained Derivative-Free Optimization

In this talk we present the algorithm (S)NOWPAC for stochastic constrained derivative-free optimization. The method uses a generalized trust region approach that accounts for noisy evaluations of the objective and constraints. To reduce the impact of noise, we fit Gaussian process models to past evaluations. Our approach incorporates a wide variety of probabilistic risk or deviation measures in both the objective and the constraints. We demonstrate the efficiency of the approach via several numerical comparisons.

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MS139

Should You Derive Or Let the Data Drive ? A Framework for Hybrid Data Driven First Principle Model Correction

Mathematical models are employed ubiquitously for description, prediction and decision making. In addressing end-goal objectives, great care needs to be devoted to attainment of appropriate balance of inexactness throughout the various stages of the underlying process. In this talk, we shall describe the interplay between model reduction and model mis-specification mitigation and provide a generic infrastructure for model re-specification based upon a hybrid first principles and data-driven approach.

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MS139

Distribution Shaping and Scenario Bundling for Stochastic Programs with Endogenous Uncertainty

We present a new approach to handle endogenous uncertainty in stochastic programs, which allows an efficient polyhedral characterization of decision-dependent probability measures and thus a reformulation of the original nonlinear stochastic MINLP as a stochastic MIP. The effectiveness of the approach will be demonstrated for stochastic network design problems, where the links are subject to random failures, as well as for stochastic project planning.

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MS139

Taming Unidentifiability of Ill-Posed Inverse Problems Through Randomized-Regularized Decision Analyses

Properties controlling groundwater flow and contaminant transport (e.g. permeability, reduction capacity, etc.) are often highly heterogeneous (spatially and temporally). Characterization of these heterogeneities using inverse methods is challenging often producing ill-posed problems with multiple plausible solutions. We have developed an approach to decision analysis that is capable of accounting for the unidentifiability of the inverse model. We present a series of synthetic decision analyses that are consistent with actual site problems.

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MS140

Numerical Approaches for Sequential Bayesian Optimal Experimental Design

How does one select a sequence of experiments that maximizes the collective value of the resulting data? We formulate this optimal *sequential* experimental design problem by maximizing expected information gain under continuous parameter, design, and observation spaces using dynamic programming. We find an approximate optimal policy via approximate value iteration, and utilize transport maps to represent non-Gaussian posteriors and to enable fast approximate Bayesian inference. Results are demonstrated on a dynamic sensor steering problem for source inversion.

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MS140

Online Optimum Experimental Design for Control Systems under Uncertainties

We have developed efficient optimal control methods for the determination of one, or several complementary, optimal experiments, which maximize the information gain about parameters subject to constraints such as experimental costs and feasibility or the range of model validity. Special emphasis is placed on evaluation of robust optimal experiments by online design of experiments, according to which the information about parameters received using online parameter estimation is used to online re-design of the running experiment.

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MS140

Bayesian Optimal Design for Ordinary Differential

Equation Models

Methodology is described for minimising the expected loss function characterising the Bayesian optimal design problem. This methodology relies on using a statistical emulator to approximate the expected loss. An extension, to consider optimal design for physical models derived from the (intractable) solution to a system of ordinary differential equations (ODEs), will also be described and illustrated on examples from the biological sciences.

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MS140

Gaussian Process based Closed-loop Bayesian Experimental Design of Computer Experiments

Using Gaussian processes as adaptive emulators for expensive computer models, a sequential optimization of the emulator (ie. with respect to utility functions like minimized prediction uncertainty) through a Bayesian experimental design approach for simulation parameter selection is investigated. The performance of several widely used utility functions and the influence of different look-ahead strategies in the Bayesian experimental design are discussed, using a plasma-wall-interaction code as real-world example.

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MS141

Scalable Methods for Optimal Experimental Design for Systems Governed by Pdes with Uncertain Parameter Fields

We formulate an A-optimal experimental design (OED) criterion for the optimal placement of sensors in infinite-dimensional nonlinear Bayesian inverse problems. We discuss simplifications required to make the OED problem computationally feasible, and present a formulation as a bi-level optimization problem whose constraints are the optimality condition PDEs defining the MAP point and the PDEs describing the action of the posterior covariance. We provide numerical results for inversion of the permeability in a groundwater flow problem.

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MS141

Efficient Particle Filtering for Stochastic Korteweg-De Vries Equations

We propose an efficient algorithm to perform nonlinear data assimilation for Korteweg-de Vries solitons. In particular we develop a reduced particle filtering method to reduce the dimension of the problem. The method decomposes a solitonic pulse into a clean soliton and small radiative noise, and instead of inferring the complete pulse profile, we only infer the two soliton parameters with particle filter. Numerical examples are provided to demonstrate that the proposed method can provide rather accurate results, while being much more computationally affordable than a standard particle filter.

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MS141

Data-Driven Spectral Decomposition and Forecasting of Ergodic Dynamical Systems

We discuss a framework for dimension reduction, mode decomposition, and nonparametric forecasting of data generated by ergodic dynamical systems. This framework is based on a representation of the Koopman operators in a smooth orthonormal basis acquired from time-ordered data through the diffusion maps algorithm. Using this representation, we compute Koopman eigenfunctions through a regularized advection-diffusion operator, and employ these eigenfunctions for dimension reduction and time integration of forecast probability densities.

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MS141

Fast Data Assimilation for High Dimensional Nonlinear Dynamical Systems

A general and fast computational framework is developed for data assimilation in high dimensional nonlinear dynamical systems. This is achieved by developing a robust probabilistic model to approximate the Bayesian inference problem and obtain samples from high dimensional posterior distributions. In addition, the proposed approach addresses one of the main challenges in uncertainty quan-

tification, namely dealing with modeling errors and their effect on inference and prediction.

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MS142

Adaptive Mesh Re-location for Randomly Fluctuating Material Fields

Stochastic models with random material fields require adaptive meshing to properly resolve the features of each (deterministic) instance at a minimum computational cost. This is a challenging issue because, to be used in as a practical tool, the cost of the error indicators and the remeshing algorithms must be very small. This discards using any a posteriori error assessment technique and precludes remeshing from scratch at each instance. We present an r-adaptivity approach for boundary value problems with randomly fluctuating material parameters solved through the Monte Carlo or stochastic collocation methods. This approach tailors a specific mesh for each sample of the problem. It only requires the computation of the solution of a single deterministic problem with the same geometry and the average parameter, whose numerical cost becomes marginal for large number of samples. Starting from the mesh used to solve that deterministic problem, the nodes are moved depending on the particular sample of mechanical parameter field. The reduction in the error is small for each sample but sums up to reduce the overall bias on the statistics estimated through the Monte Carlo scheme. Several numerical examples in 2D are presented.

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MS142

A Multilevel Control Variate Method Based on Low-Rank Approximation

Multilevel Monte Carlo (MLMC) methods are now widely used for uncertainty quantification of PDE systems with high-dimensional random data. We present a variation of MLMC, dubbed Multilevel Control Variate (MLCV), where we rely on a low-rank approximation of fine solutions from the samples of coarse solutions to construct control variates for approximating the expectations involved in MLMC. We present cost estimates as well as numerical examples demonstrating the advantage of this new MLCV approach.

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MS142

Adaptive Sde Based Sampling for Random Pde

Abstract not available.

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MS142

Computational Error Estimates for Monte Carlo Finite Element Approximation with Rough Log Normal Diffusion Coefficients

Abstract not available.

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MS143

Detecting Periodicities with Gaussian Processes

Finding an appropriate covariance function is a key issue in Gaussian process regression modelling. We discuss in this talk the construction of periodic and aperiodic covariance functions based on the RKHS framework. Furthermore, we derive a periodicity ratio using analysis of variance methods. Finally, the interest of the method is illustrated on a biology application where we identify, amongst the entire genome, the genes with a periodic activity.

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MS143

Incorporating and Learning Functional Properties Through Covariance Kernels

In Gaussian Process Modelling, a number of functional properties of the objective function can be encoded through covariance kernels. While Hilbert space expansions lead to additive decompositions of covariance kernels, we consider the issue of identifying and extracting most influencial terms of such decomposition using GP models which kernels write as sums of kernels. In particular, we focus on maximum likelihood, for which a nice property involving convexity arguments enable efficient estimation of kernel weights.

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MS143

Jointly Informative Feature Selection

We address the problem of selecting jointly informative features in the context of classification tasks. We propose several novel criteria which combine a Gaussian modelling of the features with derived bounds on their mutual information with the class. Algorithmic implementations are presented which significantly reduce computational complexity, showing that feature selection using joint mutual information is tractable. In extensive empirical evaluation these methods outperformed state-of-the-art, both in terms of speed and accuracy.

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MS143

Gaussian Process Models for Predicting on Circular Domains

We consider the framework of Gaussian process regression (or Kriging) of variables defined on circular domains. In some situations, such domains correspond to technological or physical processes involving rotations or diffusions. We introduce so-called polar Gaussian processes defined on the cylindrical space of polar coordinates, and new design of experiments on the disk. The usefulness of the approach is demonstrated on applications in microelectronics and environments.

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MS144

Uncertainty Propagation in Dynamical Systems with a Novel Intrusive Method Based on Polynomial Algebra

The paper is presenting a novel intrusive method for propagation of uncertainties in dynamical systems. The method is based on an expansion of the uncertain quantities in a polynomial series and propagation through the dynamics using a multivariate polynomial algebra. Tchebycheff and Newton basis have been used for comparison. The first one offers a fast uniform convergence, the second one a lower computational complexity. The paper details the proposed generalized algebra and illustrates its applicability.

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MS144

Multi-Fidelity Models for Flow Past An Airfoil with Operative and Geometric Uncertainties

In this work the flow past an airfoil is analysed in presence of uncertain operative conditions and geometric uncertainties with Beta-distributed perturbation. The statistics of aerodynamic performance are obtained by numerical integration. In order to reduce the computational cost of the statistical moments we use a recursive cokriging model, which exploits multi-fidelity responses, as a surrogate of aerodynamic performace on which we can perform the numerical integration.

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MS144

Sensitivity and Uncertainty Analysis in Cfd

Abstract not available.

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MS145

Data-Driven Bayesian Uncertainty Quantification for Large-Scale Problems

Abstract not available.

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MS145

Image-Based Modeling of Tumor Growth in Patients with Glioma

Abstract not available.

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MS145
Title Not Available

Abstract not available.

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MS145
Predictive Coarse-Graining

We present a Bayesian formulation to coarse-graining of atomistic systems using generative probabilistic models which allows us to address the question of quantifying epistemic uncertainty. Apart from the usual coarse-grained potential that approximates the exact free energy, the formulation is augmented with a probabilistic mapping from coarse to fine, which enables the prediction of properties in the fine-scale. The formulation allows for significant flexibility and high-dimensional parameters can be learned by sparsity-enforcing priors.

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MS146
Nonlinear Filtering with Mcmc Optimization Method

Abstract not available.

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MS146
Small Data Driven Algorithms for Solving Large-Dimensional Bsdes

We aim at solving a dynamic programming equation (inspired from BSDE) associated to a Markov chain X, using a Regression-based Monte Carlo algorithm. In order to compute the projection of the value function on a functions basis, we generate a learning sample of paths of X which is a suitable transformation of a single data set (say M historical data of X). Finally we design a data-driven resampling scheme that allows to solve the dynamic programming equation (possibly in large dimension) using only a relatively small set of M historical paths. To assess the accuracy of the algorithm, we establish non-asymptotic error estimates. Joint work with Gang Liu and Jorge Zubelli.

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MS146
Split-step Milstein Methods for Stiff Stochastic Differential Systems with Multiple Jumps

We consider stiff stochastic differential systems with Levy noise including multiple jump-diffusion processes. Such systems arise in biochemical networks that involve reactions at different time scales. They are inherently stiff and change their stiffness with uncertainty. To resolve this issue, we utilize split-step methods and investigate their convergence and stability properties. Numerical examples demonstrate the effectiveness of these methods and their ability to handle stiffness due to multiple jumps with varying intensity.

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MS146
High Accurate Methods for Coupled FBSDEs with Applications

In this talk, we will introduce accurate numerical methods, including two-step methods, multistep methods, and stochastic deferred correction methods, for solving coupled nonlinear forward backward stochastic differential equations (FBSDEs). Their high accuracy is numerically shown by their applications in solving FBSDEs, second-order FBSDEs, fully nonlinear second-order parabolic partial differential equations, and stochastic optimal control problems.

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MS147
Parameter Estimation and Uncertainty Quantification in Turbulent Combustion Computations

Bayesian inference with a model-error representation is em-

ployed to calibrate a simple chemical kinetics model for oxidation of hydrocarbon fuels in air. The model uncertainties are subsequently propagated in simulations of turbulent combustion to quantify their impact on autoignition predictions at realistic Diesel engine operating conditions. The forward propagation is performed via a non-intrusive spectral projection by computing the polynomial chaos expansion of the simulation output of interest.

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MS147

Uncertainty Inclusion and Characterization in Nonlocal Theories for Materials Modeling

Nonlocal models have been proposed in recent years to describe processes, which classical (local) models based on partial differential equations encounter challenging. Examples of this include peridynamics and nonlocal diffusion models, based on integro-differential equations, which allow the representation of evolving discontinuities in materials and of anomalous diffusion processes, respectively. These models, however, rarely account for uncertainties. Uncertainty is ubiquitous in nature. In materials modeling, uncertainty can be present in constitutive relations, material microstructure, and source terms, as well as in boundary and/or initial conditions. In this work, we propose a generalization of nonlocal models to include uncertainty in their constitutive relations and governing equations. We explore methods to quantify the effects of different types of uncertainty on the material response, for various problems of interest, and demonstrate these methods through numerical examples.

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MS147

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Abstract not available.

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MS147

Uncertainty Propagation Across Domains with Vastly Different Correlation Lengths

We develop different transmission boundary conditions that will preserve the global statistical properties of the solution across domains characterized by vastly different correlation lengths. Our key idea relies on combining local reduced-order representations of random fields with multilevel domain decomposition by enforcing the continuity of the conditional mean and variance of the solution across adjacent subdomains. The effectiveness and convergece properties of this algorithm is illustrated in numerical examples of both 1D and 2D.

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MS148

An Uncertainty Reduction Technique for Short-term Transmission Expansion Planning Based on Line Benefits

In this article we provide a novel uncertainty reduction technique to deal with uncertainties associated to Renewable Energy Sources (RES) in Transmission Expansion Planning (TEP). For the sake of simplicity, we assume the inherent uncertainty of wind and solar output are already captured in the variability of their hourly load profile. Each hourly operational state (or snapshot) of the year is assumed to represent both a realization of the uncertain RES outputs and the given time period of the year. Therefore, we handle uncertainty reduction by means of snapshot selection. Instead of taking into account all the possible operational states and their associated optimal power flow, we want to select a reduced group of them that are representative of all the ones that should have an influence on investment decisions. This reduced group of operational states should be selected to lead to the same investment decisions as if we were considering all snapshots in the target year. The reduction achieve in the size of the TEP problem should allow the user to compute an accurate enough TEP solution in a much smaller amount of time, or, alternatively, compute the expansion of the network considering more accurately other aspects of the TEP problem. Original operational states are compared in the space of candidate line marginal benefits which are relevant drivers for line investment decisions. Marginal benefits of reinforcements are computed from the nodal prices resulting from the dispatch. Principal Component Analysis (PCA) is applied to cope with the high dimension of the line marginal benefit space. Lastly, a clustering algorithm is used to group operational states with similar marginal benefits together. Our algorithm has been tested on a modified version of the standard IEEE 24 bus system.

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MS148

Quasi-Monte Carlo Methods Applied to Stochastic Energy Optimization Models

We consider two-stage stochastic unit commitment models for electricity production and trading and study the use of Quasi-Monte Carlo (QMC) methods for scenario generation. We provide conditions on the optimization model and the underlying probability distribution implying that QMC error analysis applies approximately to two-stage mixed-integer integrands. Hence, convergence rates close to the optimal O(1/n) may be achieved. Numerical results are presented for two particular randomized QMC methods that show their superiority to classical Monte Carlo.

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MS148

Scalable Algorithms for Large-Scale Mixed-Integer Optimization Problems in Ac Power Systems

We propose a method that solves constrained optimization problems over AC power distribution systems over mixed set of variables, where discrete variables model state of power transformers or state of tap changers. Although these problems are mixed-integer non-linear programs, they can be solved over radial networks by a fully polynomial-time approximation scheme. The reason is that our method takes advantage of the radial structure of the network and outputs an approximate optimal solution in time that is polynomial both in the network size and in the approximation factor. Our solution technique is based on the Belief-Propagation (BP) algorithm that has been successfully applied in the past to solve discrete problems in statistical physics, machine learning and coding theory. The main challenge that we need to overcome to apply BP techniques lies in extending it to problems with continuous variables, and specifically to voltage and flow variables in the power flow equations. We also discuss possible extensions of the BP techniques, through construction of a hierarchy of BP-based LP relaxations, to the related problems of transmission level problems over loopy networks.

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MS148

Probabilistic Forecasting of Wind and Solar Power Using Epi-Splines

We introduce a non-parametric density density estimation method based on recently introduced epi-spline bases, which we use to characterize forecast error distributions for real-world wind and solar power production in electric power systems. We discuss scenario generation methods based on these density estimates, and characterize both the mean and probabilistic forecast accuracy on real-world data sets from the Bonneville Power Administration and the California Independent System Operator.

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MS149

Model Order Reduction of Linear Systems Driven by Levy Noise

We discuss model order reduction for linear dynamical systems driven by Levy processes. In particular, we investigate balanced truncation and singular perturbation approximation for these systems. These methods are known to come with computable error bounds and to preserve stability in the deterministic setting. We will discuss in how far these properties carry over to the stochastic case, and we will derive H_2-type error bounds. Numerical experiments illustrate our findings.

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MS149

ADM-CLE Approach for Detecting Slow Variables

in Continuous Time Markov Chains and Dynamic Data

A method for detecting intrinsic slow variables in high-dimensional stochastic chemical reaction networks is developed and analyzed. It combines anisotropic diffusion maps (ADM) with approximations based on the chemical Langevin equation (CLE). The resulting approach, called ADM-CLE, has the potential of being more efficient than the ADM method for a large class of chemical reaction systems. The ADM-CLE approach can be used to estimate the stationary distribution of the detected slow variable, without any a-priori knowledge of it.

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MS149

Balanced Truncation of Stochastic Linear Control Systems

We consider two approaches to balanced truncation of stochastic linear systems, which follow from different generalizations of the reachability Gramian of deterministic systems. Both preserve mean-square asymptotic stability, but only the second leads to a stochastic H^∞-type bound for the approximation error of the truncated system.

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MS150

On a Connection Between Adaptive Multilevel Splitting and Stochastic Waves

Adaptive Multilevel Splitting (AMS for short) is a general Monte-Carlo method to simulate and estimate rare events. In the framework of molecular dynamics, this technique can for example be used to generate reactive trajectories, namely equilibrium trajectories leaving a metastable state and ending in another one. In this talk, we will present a connection between AMS and stochastic waves, i.e. the transformation of a Markov process by a random time change. In particular, this connection allows us to analyze AMS as a Fleming-Viot type particle system.

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MS150

Pseudogenerators for Under-Resolved Molecular Dynamics

Many features of molecules which are of physical interest (e.g. molecular conformations, reaction rates) are described in terms of its dynamics in configuration space. We consider the projection of molecular dynamics (governed by a stochastic Langevin equation) in phase space onto configuration space. We review the Smoluchowski equations as overdamped limit, and show that for small times a Smoluchowski equation, scaled non-linearly in time, governs the evolution of the configurational coordinate even for general damping.

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MS150

The Parallel Replica Algorithm: Mathematical Foundations and Recent Developments

I will present the parallel replica algorithm, which is an accelerated dynamics method proposed by A.F. Voter in 1998. The aim of this technique is to efficiently generate trajectories of a metastable stochastic process. Recently, we propose a mathematical framework to understand the efficiency and the error associated with this technique. Generalizations of the original method in order to widen its applicability have been proposed. References: D. Aristoff, T. Lelivre and G. Simpson, The parallel replica method for simulating long trajectories of Markov chains, AMRX, 2, 332-352, (2014) A. Binder, T. Lelivre and G. Simpson, A Generalized Parallel Replica Dynamics, Journal of Computational Physics, 284, 595-616, (2015). C. Le Bris, T. Lelivre, M. Luskin and D. Perez, A mathematical formalization of the parallel replica dynamics, Monte Carlo Methods and Applications, 18(2), 119146, (2012).

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MS150

Generalizing Adaptive Multilevel Splitting

(Adaptive) Multilevel Splitting methods are standard rare event simulation techniques, considered her for events e.g. of the form $\{\tau_A \leq \tau_B\}$ where τ_A and τ_B are hitting times of some given simulable random process. The method is basically a multiple replicas method where (i) replicas' paths are stored; (ii) some replicas are duplicated depending on some given level function; and (iii) new replicas dynamics are re-simulated with the original true dynamics, starting from the state associated with the reached considered level. In this talk, we will give a theoretical framework giving conditions under which this type of methods (with possibles generalizations and variants) are indeed consistent (i.e. here yielding unbiased estimator of the associated rare event probability).

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MS151

Linear Collective Approximations for Parametric and Stochastic Elliptic Pdes

Consider the elliptic problem $-\operatorname{div}\Big(a(y)\nabla u(y)\Big) = f$ in $D \subset \mathbb{R}^m$ parametrized by $y \in \mathbb{I}^\infty := [-1,1]^\infty$ with $u(y)|_{\partial D} = 0$ and affine parametric dependence of $a(y)$. If there is a sequence of approximations in $H_0^1(D)$ to one solution $u(y_0)$ at $\forall y_0 \in \mathbb{I}^\infty$, with an error convergence rate, we proved by linear collective methods that it induces a sequence of approximations to the solution $u(y)$ as a mapping from $\mathbb{I}^\infty$ to $H_0^1(D)$ in the norm of $L_\infty\Big(\mathbb{I}^\infty, H_0^1(D)\big)$ with the same error convergence rate.

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MS151

Applying Quasi-Monte Carlo to an Eigenproblem with a Random Coefficient

In this talk we look at applying finite elements (FE) and quasi-Monte Carlo (QMC) methods to an elliptic eigenproblem with a random coefficient where the aim is to approximate the expected value of the principal eigenvalue and linear functionals of the corresponding eigenfunctions. By formulating the expected values as integrals we are able to apply QMC quadrature to the FE approximations. We show that the principal eigenvalue and linear functionals of the corresponding eigenfunction, also their respective FE approximations, belong to the spaces required for the QMC theory and provide numerical results.

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MS151

Novel Monte Carlo Approaches for Uncertainty Quantification of the Neutron Transport Equation

Neutron Transport is an important problem in reactor physics, a six dimensional integro-differential equation that is extremely costly to solve. Moreover, the geometry and the coefficients, known as cross-sections, are typically uncertain. Quantifying these uncertainties is a formidable task even in simple toy problems. Using Novel ideas, such as lattice rules (QMC) and multilevel simulation, Monte Carlo methods can be speeded up significantly. We confirm this numerically and by exploring the background theory.

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MS151

Sparse-Grid Quadrature for Elliptic Pdes with Log-Normal Diffusion

Elliptic boundary value problems with log-normally distributed diffusion coefficients arise, for example, in the modelling of subsurface flows in porous media and can be written in divergence form

$$-\operatorname{div}(a(x,\omega)\nabla u(x,\omega)) = f(x).$$

The method of choice to deal with these equations mainly depends on the quantities of interest which usually arise as high-dimensional integrals. In many cases, the integrand does not depend equally on each dimension. This anisotropy can be exploited to construct sparse-grid quadrature methods. In order to analyze the convergence of these methods, it is important to establish sharp bounds on the number of indices contained in anisotropic index sets.

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MS152

Optimal Bayesian Design of the Oral Glucose Tolerance Test Using An Ode Model

The Oral Glucose Tolerance Test (OGTT) is routinely performed in health units around the world as a tool to diagnose Diabetes related conditions. The test is done in fasting after a night sleep and blood glucose is measured at arrival. The patient is then asked to drink a sugar solution and thereafter blood glucose is measured at 1, 1.5 and/or 2h depending on local practices. The profile at which blood glucose increases and in the course of the test is controlled to return (or not return) to normal levels should provide health specialists with a diagnosis. However, current data analyses are limited and a better approach is required to obtain a greater value for the OGTT. We have developed a model based on a system of ODE's which fits the OGTT data well in many cases. Bayesian inference is used to estimate three parameters that are directly related to the Glucose/Insulin system and provide a basis for a more comprehensive diagnosis. In this talk we discuss a further problem on designing the blood sampling times to maximize the information obtained by the OGTT with the same number of samples or with 1 or 2 more samples, to provide a far more reliable result while adding only marginal costs. We maximize the expected gain in the information from data using a MCMC estimator embedded in a stochastic optimization procedure.

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MS152

Efficiency and Computability of MCMC with Autoregressive Proposals

We analyse computational efficiency of Metropolis-Hastings algorithms with stochastic AR(1) process proposals. These proposals include, as a subclass, discretized Langevin diffusion (e.g. MALA) and discretized Hamiltonian dynamics (e.g. HMC). We extend existing results about MALA and HMC to target distributions that are absolutely continuous with respect to a Gaussian where the covariance of the Gaussian is allowed to have off-diagonal terms.

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MS152

Fast Solutions to Large Linear Bayesian Inverse Problems

Matrix splittings and polynomials, well established iterative techniques from numerical linear algebra, can optimally accelerate the geometric convergence rate of Gibbs samplers used to solve large Bayesian linear inverse problems. This approach is used to solve a linear model of the heights of pathogenic biofilms on medical devices, before and after anti-microbiocide treatments, from 3-D movies generated by a confocol scanning laser microscope. Limitations of the linear approach are overcome by solving a pixel-based Bayesian non-linear model.

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MS153

Probability Measures for Numerical Solutions of Deterministic Differential Equations

Abstract not available.

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MS153

Correction of Model Reduction Errors in Simulations

This talk presents an approximation error approach for correction of the approximation errors in reduced simulation models. Here, the approximation error is modelled as an additive error and approximated using a low-cost predictor model which predicts the approximation error for given simulation input parameters. The approximation error approach is tested with different simulation models and the accuracies and computation times of the models with and without the approximation error correction are compared.

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MS153

Confidence in Bayesian Nonparametrics? Some Mathematical (frequentist) Facts

There has been substantial progress in the last few years about when posterior based inference has objective justifications in situations where the Bayesian model sits on an infinite dimensional parameter (such as a regression function or density). I will discuss some of the main findings, ideas, conclusions and perspectives.

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MS153

The von Neumann-Morgenstern Approach to Choice Under Ambiguity: Updating

A choice problem is risky (ambiguous) if the decision maker is choosing between probability distributions (sets of probability distributions) over utility-relevant consequences. Continuous linear preferences over sets of probabilities extend expected utility preferences and deliver: first- and second-order dominance for ambiguous problems; complete separations of attitudes toward risk and ambiguity; new classes of preferences that allow decreasing relative ambiguity aversion; and a complete and dynamically consistent theory of updating convex sets of priors.

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MS154

Compositional Uncertainty Quantification for Coupled Multiphysics Systems

In goal-oriented design and analysis processes for coupled multiphysics systems, we often have available several information sources that vary in fidelity. To optimally exploit these sources of information, we develop a compositional offline/online uncertainty quantification methodology using a combination of ensemble Gibbs sampling and sequential importance resampling. This approach enables the efficient evaluation of information source discrepancy sensitivities associated with system level quantities of interest. We demonstrate our methodology on a coupled aero-structural system.

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MS154

Multifidelity Uncertainty Propagation in Multidisciplinary Systems

The objective of this work is to tackle the complexities involved with uncertainty propagation in feedback coupled multidisciplinary systems. We present a multifidelity approach with adaptive sampling for updating low-fidelity models to achieve efficient uncertainty propagation that exploits the structure of the multidisciplinary system. The low-fidelity prediction and its uncertainty are used to select additional designs to evaluate, so as to selectively refine each of the disciplinary low-fidelity models.

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MS154

Model Selection Under Uncertainty: Coarse-Graining Atomistic Models

Issues in modeling and simulation of reduced-order models include model selection, calibration, validation, and error estimation, all in the presence of uncertainties in the data, prior information, and the model itself. These issues are addressed via the Occam-Plausibility ALgorithm (OPAL), which chooses, among a large set of models, the simplest valid model that may be used to predict chosen quantities of interest. An illustrative example application to coarse-grained models of atomistic polyethylene is given.

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MS154

Data-Driven Distributionally Robust Optimization Using the Wasserstein Metric

We consider stochastic programs where the distribution of the uncertainties is only observable through a training dataset. Using the Wasserstein metric, we construct a ball in the space of probability distributions around the empirical distribution, and we seek decisions that perform best in view of the worst-case distribution within this ball. We demonstrate that the resulting distributionally robust optimization problems can be reformulated as finite convex programs and that their solutions enjoy powerful finite-sample guarantees.

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MS155

Optimal Experimental Design using Multi Level Monte Carlo with application in Composite Material Damage Detection

Composite materials can be produced by a number of techniques, which aim to combine plies of fiber in different directions. Composites can be degraded by a number of mechanisms. Detection of defects in composites such that delamination can be addressed by Electrical Impedance Tomography (EIT). The electrical impedance problem is to recosntruct the conductivity field in the material based on the voltage measurements collected on the electrodes placed on the boundary. In a Bayesian framework, we infer the presence of delamination based on the posterior conductivity field. We present a Multi-Level Monte Carlo (MLMC) approach for the integration of the posterior conductivity field and perform a comparative analysis with some accelerative methods such that the Laplace method.

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MS155

Optimal Experimental Design for Geophysical Imaging of Flow in Porous Media

Designing experiments for imaging fluid flow requires the integration of the dynamical system describing the flow, the geophysical imaging technique, and historic data. In this talk we explore optimal experimental design methods for such problems, and demonstrate the applicability of the techniques for the problem of imaging subsurface flow using seismic methods.

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MS155

Optimal Electrode Positions in Electrical

Impedance Tomography

The aim of electrical impedance tomography is to recover information about the conductivity inside a physical body from boundary measurements of current and voltage. In practice, such measurements are performed with a finite number of electrodes. This work considers finding optimal positions for the electrodes within the Bayesian paradigm based on available prior information; the goal is to place the electrodes so that the posterior density of the (discretized) conductivity is as localized as possible.

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MS155

Using Topological Sensitivity and Reachability Analysis Large Model Spaces

It is common fallacy to assume that models that fit data and our prior expectations must be good. Here we show, focussing on dynamical systems, how we start to asses how many models can fit a given data set. And we will discuss Bayesian and control engineering approaches to (i) determine experimental conditions that are likely to discriminate between such plausible models; or (ii) allow us to analyze ensembles of models jointly.

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MS156

Adaptive Data Assimilation Scheme for Shallow Water Simulation

Data assimilation is the process of optimally combining the estimated forecast states and the observations to obtain a better representation of the system states. In most DA methods, the assimilation occurs whenever the observations become available. For many high dimensional and nonlinear forecast problems, this has become inefficient. We present an adaptive data assimilation scheme to control the assimilation frequency. The control criteria will be discussed together with numerical tests on the shallow water equations.

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MS156

A Statistical Analysis of the Kalman Filter

Kalman filters present several methodological problems because analytical results focus on their exponential convergence. Therefore, such methods have difficulties in estimating static parameters, in assimilating general data models, and in finding utility in resource constrained scenarios. In this work, we replace the deterministic assumptions in previous analyses with more natural probabilistic ones. Consequently, (1) we demonstrate that the Kalman Filter converges for a robust choice of tuning parameters and (2) we present a new theoretical foundation for stopping criteria for a prescribed precision level. A static parameter algorithm is developed and extensions to low-memory constraints, rank-deficient problems, and general data models are suggested. The concepts are demonstrated on a large data set from the Center of Medicare and Medicaid.

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MS156

Dynamic Parameter and State Estimation for Power Grid Systems

We consider the problem of dynamic state and parameter estimation for large-scale power grid systems. The goal is to determine the most likely parameters and/or dynamic states based on fast-rate measurements available from phase measuring units (PMUs). We will present the inversion for generators inertia under transients caused by large disturbances in the load. For this we developed an optimization-based framework that uses state-of-the-art parallel forward and adjoint numerical integration.

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MS157

Adaptive Algorithms Driven by A Posteriori Estimates of Error Reduction for PDEs with Random Data

We present an efficient adaptive algorithm for computing stochastic Galerkin finite element approximations of elliptic PDEs with random data. Our adaptive strategy is based on computing two error estimators associated with two distinct sources of discretisation error. These estimators provide effective estimates of the error reduction for enhanced approximations. The algorithm adaptively 'builds' a polynomial space over a low-dimensional manifold of the parameter space so that the total discretisation error is reduced in an optimal manner.

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MS157

Optimal Approach for the Calculation of Stochastically Homogenized Coefficients of Elliptic Pdes

The calculation of effective coefficients of stochastic elliptic PDEs involving multiple length scales is a computationally intensive task. In this talk, we give error estimates for the three types of error (discretization, statistical, finite domain) and model the computational work. Then we minimize the work for a given error. This approach allows to find an optimal balance between fineness of the spatial discretization, the number of samples, and the size of the spatial domain.

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MS157

Goal-Oriented Error Control in Low-Rank Approximations

Abstract not available.

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MS157

Goal-Based Anisotropic Adaptive Control of Stochastic and Deterministic Errors

A strategy for goal-oriented error estimation of the coupled deterministic and stochastic approximation errors is proposed in this paper. Furthermore, an adaptive anisotropic method is proposed to enhance the quality of a functional of interest obtained by the coupled stochastic-deterministic solution of a parametrised system. The anisotropy in the deterministic space is controled for a functional of interest via a riemannian metric (hessian) based method and a similar approach is extended to stochastic errors. The proposed approach is applied to computational fluid dynamics problems modeled by Euler and Navier-Stokes equations, where we considered up to two uncertain parameters.

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MS158

Bayesian Screening Through Gaussian Processes Hyper-Parameter Sampling

Gaussian processes have proven to be powerful emulators of expensive numerical models. Kernels with auto relevance determination use the Gaussian process' hyper-parameters for screening input variables. This is commonly done through their maximum likelihood estimates, which might be prone to underestimating the complexity of the correlation structure. In this work, we propose a Bayesian scheme akin to sequential sampling for a probabilistic estimation of the maximum a posteriori candidates.

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MS158

Combining Feature Mapping and Gaussian Process Modelling in the Context of Uncertainty Quantification

Uncertainty Quantification (UQ) and Machine Learning (ML) are two rapidly growing research topics that aim at the solution of similar problems from different perspectives and methodologies. This contribution explores the potential of using Kriging-based surrogate models as advanced learners, combined with unsupervised learning algorithms based on the deep learning paradigm. The effectiveness of the approach is evaluated on several benchmark applications in both UQ and ML.

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MS158

Single Nugget Kriging: Better Predictions at the Extreme Values

We propose a method with better predictions at extreme values than the standard method of Kriging. We construct our predictor in two ways: by penalizing the mean squared error through conditional bias and by penalizing the conditional likelihood at the target function value. Our prediction exhibits robustness to the model mismatch in the covariance parameters, a desirable feature for computer simulations with a restricted number of data points.

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MS158

Modelling Faces in the Wild with Gaussian Processes

Face verification has been studied extensively and become one of the most active research topics in computer vision. However, various visual complications remain challenging for robust face verification when face images are taken in the wild. On the other hand, Gaussian process models as the representatives of Bayesian nonparametric models can cover the intrinsically complex variations. In this talk, we present how to model faces in the wild using Gaussian processes.

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MS159

An Adaptive Strategy on the Error of the Objective Functions for Uncertainty-Based Derivative-Free Optimization

In this work, a strategy is developed to deal with errors affecting the objective functions in uncertainty-based optimization. It relies on the exchange of information between the outer loop based on the optimization algorithm and the inner uncertainty quantification loop. In the inner loop, a control is performed to decide whether a refinement for the current design is appropriate or not. Then, an accurate estimate of the objective function is done only for non-dominated solutions.

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MS159

Parameter Calibration and Optimal Experimental Design for Shock Tube Experiments

A Bayesian framework for parameter inference and optimal experimental design is developed. The formalism explicitly accounts for the impact of uncertainty in experimental operating conditions during which data is collected, and of measurement errors. Implementation of the framework is illustrated in light of applications to (i) the inference of reaction rates and the parametrization of rate laws based on time-resolved, noisy measurements of species concentrations, and (ii) the optimal design of shock tube experiments.

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MS159

Coordinate Transformation and Polynomial Chaos for the Bayesian Inference of a Gaussian Process with Parametrized Prior Covariance Function

This work concerns the Bayesian inference of fields from Gaussian priors with parametrized covariance. The problem is classically made finite by Karhunen-Loève decompositions over covariance-parameters dependent bases. We propose instead to use a fixed basis and account for covariance-parameters dependences through the coordinates prior. Sampling the posterior is also accelerated by constructing polynomial surrogates in the global coordinates. The approach is demonstrated and illustrated on the inference of spatially-varying log-diffusivity fields from noisy data.

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MS159

Representation of Model Uncertainty in Space Debris Orbit Determination with Sparse Measurements

This paper presents a new method to capture unmodelled components in orbital mechanics with application to the orbit determination of space debris. The approach proposed in this work uses a polynomial expansion in the state space with stochastic coefficients. The distribution of the coefficients is recovered from the minimisation of an uncertainty measure in the space of the stochastic coefficients so that the resulting flow is contained in the confidence intervals provided by the measurements.

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MS160

Statistical Approaches to Forcefield Calibration and Prediction Uncertainty in Molecular Simulation

The important development of molecular simulation in the past decades has made it a very attractive tool for the study of condensed matter. It is now commonly used to predict thermophysical properties of fluids. The use of molecular simulation as a predictive tool requires to estimate the uncertainty associated with the predicted value for a property. The simulation results uncertainty arising from the forcefield has long been ignored. The forcefield contains all the information about the potential energy of a system, coming from interatomic interactions, which are encrypted in parameters commonly calibrated in order to reproduce some experimental data. It is only very recently that careful investigations of the effect of forcefield parameters uncertainties have been undertaken [Rizzi et al, MMS 2012; Angelikopoulos et al, JCP 2012; Cailliez and Pernot, JCP 2011]. This is mainly due to the difficulty to estimate forcefield parameters uncertainties, that necessitates an extensive exploration of parameter space, incompatible with the computer time of molecular simulations. In recent years, we have explored various calibration strategies and calibration models within the Bayesian framework [Kennedy and O'Hagan, Roy. Stat. Soc. B, 2001]. We have studied a two-parameters Lennard-Jones potential for Argon, for which the calibration can be done using cheap analytical expressions. We have shown that prediction uncertainty is larger than characteristic statistical simulation uncertainty [Cailliez and Pernot, JCP 2011]. For more complex systems, more parameters have to be calibrated and, in absence of analytical models, the calibration process requires to run long molecular simulations. In order to face these issues, we have used kriging metamodels and optimal infilling strategies to limit the number of molecular simulations to be performed during the calibration process. We have benchmarked this methodology on the water TIP4P forcefield [Cailliez et al, JCC 2014].

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MS160

Mapping the Structural and Alchemical Landscape of Materials, from Molecules to the Condensed Phase

Abstract not available.

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MS160

Modeling Material Stress Using Integrals of Gaussian Markov Random Fields

Material scientists are interested in the variability of stress conditions as compressive forces are applied throughout a volume. Sophisticated computer codes are used to simulate von Mises stress-fields, and it is often observed that the internal grain boundary structure is important. We describe the stress-field within a realized cube of tantalum (having tens of grains and ¿570,000 computational elements) with a model featuring integrals of GMRFs on second- and third-order grain boundaries.

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MS160

Multiscale Modeling of with Quantified Uncertainties and Cloud Computing: Towards Computational Materials Design

Abstract not available.

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MS161

Gradient Projection Method for Stochastic Optimal Control in Finance

Abstract not available.

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MS161

Multi-symplectic Methods for Stochastic Maxwell Equations

Abstract not available.

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MS161

Error Estimates of the Crank-Nicolson Scheme for Solving Decoupled Forward Backward Stochastic Differential Equations

Abstract not available.

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MS161

Stochastic Optimization with Bsdes

Abstract not available.

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MS162

Active Subspaces and Reduced-Order Models for High-Dimensional Uncertainty Propagation

Recent work from our team in the application of active subspaces and reduced-order models to the problem of forward propagation of uncertainties in systems governed by the solution of partial differential equations are discussed. The methods enable us to discover low-dimensional manifolds that, together with other advanced UQ techniques result in greatly improved capabilities. Examples from an aerothermal nozzle problem are presented and discussed.

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MS162

Title Not Available

Abstract not available.

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MS162

Global Sensitivity Analysis with Correlated Variables

This work will highlight challenges posed by input correlation in traditional variance based global sensitivity analysis. We will present semi-analytical approaches to compute global sensitivity metrics in the presence of input correlation. The proposed methods will be compared on jet engine applications where sensitivities of both uncalibrated and calibrated models are desired with respect to prior and posterior distributions respectively. Finally, we will also present the use of novel visualization techniques to understand structural and correlative sensitivity in high dimensions.

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MS162

Overview of New Probabilistic Characteristics: Cvar Norm and Buffered Probability of Exceedance (bpoe)

This paper overviews two new probabilistic characteristics: 1) Stochastic CVaR Norm, and 2) Buffered Probability of Exceedance (bPOE). Stochastic CVaR norm is a parametric function measuring distance between two random values. We have used this norm for building new algorithms for approximating distributions (e.g., a discrete distribution by some other discrete distribution). bPOE counts tail outcomes averaging to some specific threshold value. Minimization of bPOE can be reduced to Convex and Linear Programming.

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MS163

Surrogate-based Approach for Optimization Problems under Uncertainty

We propose a general surrogate model approach to tackle optimization problems under uncertainty. We then show that the proposed surrogate models are equivalent to both robust and distributionally robust optimization models, provided an appropriate selection of model parameters. Finally, we present computational experiments that highlight the efficiency of the surrogate model approach.

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MS163

Comparison of Stochastic Programming and Ro-

bust Optimization Approaches for Risk Management in Energy Production

In this talk, we compare three optimization methods to solve an operational decision-making problem. The methods involve stochastic programming, robust optimization, and a third hybrid method. The uncertainty is represented by finite number of discrete scenarios and convex uncertainty sets, while the risk management is addressed using CVaR and a budget uncertainty constraint. The methods use an efficient parallelization of Benders Decomposition. We compare the algorithmic implementation of the methods, their performance and operational results.

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MS163

Security and Chance Constrained Unit Commitment with Wind Uncertainty

With increasing wind energy penetration, power system operators are interested in cost-efficient operation of transmission grids and securing them against random component failures. Moreover, the presence of stochastic wind generation alters the traditional methods for solving the day-ahead unit commitment. Hence, we formulate the stochastic multi-stage Security and Chance Constrained Unit Commitment problem under wind uncertainty and discuss methods to reformulate into a tractable form and further propose decomposition algorithms to obtain optimal solutions for relatively large problems.

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MS163

Spatio-Temporal Hydro Forecasting of Multireservoir Inflows for Hydro-Thermal Scheduling

Hydro-thermal scheduling is the problem of finding an optimal dispatch of power plants in a system containing both hydro and thermal plants. Since hydro plants are able to store water over long time periods, and since future inflows are uncertain due to precipitation, the resulting multi-stage stochastic optimization problem becomes challenging to solve. Several solution methods have been developed over the past few decades to compute practically useful operation policies. One of these methods is stochastic dual dynamic programming (SDDP). SDDP poses strong restrictions on the forecasting method generating the necessary inflow scenarios. In this context, the current state-of-the-art in forecasting are periodic autoregressive (PAR) models. We present a new forecasting model for hydro inflows that incorporates spatial information, i.e., inflow information from neighboring reservoirs of the system, and that also satisfies the restrictions posed by SDDP. We benchmark our model against a PAR model that is similar to the one currently used in Brazil. Three multi-reservoir basins in Brazil serve as a case study for the comparison. We show that our approach outperforms the benchmark PAR model and present the root mean squared error (RMSE) as well as the seasonally adjusted coefficient of efficiency (SACE) for each reservoir modeled. The overall decrease in RMSE is 8.29% using our approach for one month-ahead forecasts. The decrease in RMSE is achieved without additional data collection while only adding 11.8% more state variables for the SDDP algorithm.

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MS164

Theory and Applications of Random Poincare Maps

For deterministic ODEs, Poincaré maps (also called return maps) are useful to find periodic orbits, determine their stability, and analyse their bifurcations. The concept of Poincaré map naturally extends to the case of irreversible stochastic differential equations, where it takes the form of a discrete-time, continuous-space Markov chain. We present spectral-theoretic results allowing to quantify the metastable long-term dynamics of these processes. Applications include the description of the interspike interval for the stochastic FitzHugh–Nagumo equation and the asymptotic computation of the distribution of first exits through an unstable periodic orbit.

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MS164

Dynamic Model Reduction for Stochastic Chemical

Reaction Systems with Stiffness

The research on reduction methods is driven by the complexity of chemical reaction systems, 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. In this work we propose an algorithm based on the theory of stochastic singular perturbation, that can be applied to stochastic reaction systems with stiffness, to obtain their random low-dimensional manifolds.

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MS164

Stochastic Effects and Numerical Artefacts in Pure and Mixed Models in Biology

Biological systems consist of coupled processes occurring at multiple time- and space-scales. Choosing a suitable pure model at a fixed scale, coupling different pure models to form a mixed (hybrid) model, and choosing numerical methods for such models, are generally not straightforward tasks. In this talk, stochastic effects and numerical artefacts, playing an important role in the model building, are analysed using numerical analysis, and dynamical systems, chemical reaction and perturbation theory.

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MS165

Probabilistic Analysis of a Rock Salt Cavern with Application to Energy Storage System

This study provides a probabilistic analysis of a typical renewable energy storage cavern in rock salt. An elasto-viscoplastic-creep constitutive model is applied to a numerical model to assess its mechanical behavior. Sensitivity measures of different variables are computed by global sensitivity analysis. The propagation of parameter uncertainties and failure probability are evaluated by utilizing a Monte-Carlo based simulation. Surrogate modeling technique is applied to reduce required computational time and effort in probabilistic analysis.

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MS165

Efficient Estimation of Saturation Distribution in Stochastic Two-Phase Flow Problems

We introduce an efficient distribution method to estimate the full distribution of saturation in two-phase flow problems with random (uncertain) permeability and porosity fields. We demonstrate how accurate and inexpensive the estimation is compared to direct Monte Carlo simulation, even with large variances or small correlation lengths. Finally, we discuss the notion of quantiles for the saturation and illustrate how the distribution method can directly lead to this comprehensive way of managing flow scenarios under uncertain conditions.

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MS165

Tracer Dispersion in a Realistic Field Case with the Polar Markovian Velocity Process (PMVP) Model

For the quantification of tracer dispersion uncertainty, the recently developed PMVP model employs a Markov process for the Lagrangian velocity of tracer particles. In this work, we evaluate the performance of the PMVP model for a realistic testcase that is defined by the well-known MADE 2 benchmark. Confirming our previous results, we find accurate model predictions and analyze in great detail remaining differences between the reference data and our PMVP predictions.

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MS165

Uncertain CO_2 Transport in Large-Scale Carbon Capture and Storage

Numerical simulation of migration of CO_2 in subsurface storage reservoirs is computationally demanding due to the large ranges of spatial and temporal scales, as well as the uncertainty in the physical input parameters. Efficient representation of the uncertainties is challenging due to the hyperbolic nature of the governing equations. A reduced-order stochastic Galerkin method by means of locally discarding insignificant chaos modes is presented together with test cases from the North Sea.

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PP1

Ridge-Scad Quantile Regression Model for Big Data

Extraction of useful information from massive data sets is a big challenge for statisticians and researchers. Moreover, sample correlation becomes very high in case of huge number of variables. The usual linear regression and quantile regression models are failed to resolve these issues. Therefore, the Ridge-SCAD quantile variable selection technique is developed and the model selection consistency is established. The proposed model showed better performance as compared to the available models in the simulations studies.

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PP1

A Bayesian View of Doubly Robust Causal Inference

In causal inference, propensity score methods rely on the modelling of the assignment to treatment. Such an approach is difficult to justify from a Bayesian setting, since the treatment assignment model can play no part in likelihood-based inference for outcome. We propose a Bayesian posterior predictive approach in the framework of misspecified models to construct doubly robust estimation procedures, which require only one of the exposure and outcome models to be correctly specified.

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PP1

Padé Approximation for the Helmholtz Equation with Parametric Or Stochastic Wavenumber

We study the Helmholtz problem with parametric or stochastic wavenumber k^2, varying in $K \subset \mathbb{R}^+$ (interval of interest). We introduce the solution map $\mathcal{S}$, which to $k^2 \in K$ associates $u(k^2, x)$, solution of the Helmholtz problem. We extend $\mathcal{S}$ to $\mathbb{C}^+ := \mathbb{R}_{>0} + i\mathbb{R}$, obtaining a meromorphic map with a simple pole in each $\lambda \in \Lambda$, Λ being the set of eigenvalues of the Laplacian. A rational Padé approximant of $\mathcal{S}$ is constructed, and upper bounds for the approximation error are derived.

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PP1

Effective Emulators for Flood Forecasting and Realtime Water Management

We present the development of a Gaussian process (GP) based mechanistic emulator of a nonlinear model used for the control of water in urban drainage networks. The GPs covariance function corresponds to a linear model: an efficient heuristic proxy for the nonlinear dynamics. The mapping between the parameters of the linear and nonlinear model is learned from data generated by the latter. Small generalization errors of the emulator confirm the adequacy of the datadriven proxy.

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PP1

Identification of Physical Parameters Using Gaussian Process Change-Point Kernels

Various physical systems are approximated by a linear domain near the equilibrium and a non-linear domain where the approximations wear off. Gaussian Processes are nonparametric, Bayesian models giving relationship between measured points in terms of mean and variance. In this poster we apply a change-point kernel to parametrize the Gaussian Process and learn values of required physical parameters by maximizing marginal likelihood. Our method will be used to learn Youngs modulus from Experimental data.

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PP1

Quantifying the Effect of Parameter Uncertainty in the Output of a Microsimulation Model of Cancer: The Case of Overdiagnosis in Prostate Cancer

Estimates resulting from microsimulation models of cancer have substantial parameter uncertainty. We analyze its effect with probabilistic sensitivity analyses. This is not feasible since, number of parameters is large and running time is high. We minimize model runs by running it at a limited number of points, and use the resulting data to fit a Gaussian Process emulator. Even for a computationally expensive model, we show it is possible to analyze parametric uncertainty.

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PP1

Uncertainty Quantification from a Hierarchy of Models

There are different ways to classify uncertainty or its sources. The most common distinction is to divide them into two types: random uncertainty and epistemic uncertainty. The first is considered as non reducible due to the natural variability of a random phenomena. The second is caused by a lack of knowledge which can be reduced by acquiring more information. In this paper we argue that the parameters involved in the physical equations and their numerical implementation can not be considered to be random quantities. Our approach is to closely examine the use of classification technics in a deterministic uncertainty quantification method. Each output obtained with fixed parameters is assimilated to a response of the model. The set of parameters and the response obtained using this set will be named indifferently "candidate". The idea is then to sort the candidates according to a level of adequacy, named "score", with a set of preset measurements. This approach can be seen as an attempt to produce a score associated with every theoretical model (candidate) or as a protocol to refute evaluation or experimental measurements. Once the outputs are scored, the candidates are weighted according to their score value to estimate the covariance matrix.

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PP1

Demonstration of Uncertainty Quantification Python Laboratory (UQ-PyL)

Uncertainty Quantification Python Laboratory (UQ-PyL) is a software platform that integrates many kinds of uncertainty quantification (UQ) methods, including experimental design, statistical analysis, sensitivity analysis, surrogate modeling and parameter optimization. It is designed for uncertainty analysis and parameter optimization of large complex dynamical models. This poster describes the design structure and illustrates the main features of the software, which can be downloaded from http://uq-pyl.com.

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PP1

Uncertainty Propagation in Flooding Using Non-Intrusive Polynomial Chaos

Uncertainty propagation of initial conditions and atmospheric forcings using the coupled hydrologic/hydrodynamic tRIBS model suite. A polynomial chaos expansion with non-intrusive spectral projection is used for uncertainty propagation and global sensitivity analysis to quantify the influence of input parameters and forcings on flooding extent in test cases and experimental setups for rainfall-runoff processes.

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PP1

Estimation of Smooth Functions with An Application to Climate Extremes

We develop a new and general statistical methodology for estimating smooth functions. The optimization is based on a reliable numerical procedure which is fast, stable and efficient. The approach deals with fitting flexible models of random variables that are independent but not identically distributed. This flexibility addresses any prior information depending on covariates. For illustration, we apply the method to a non-stationary Generalized Extreme Values distribution, while incorporating a smooth structure using Generalized Additive Models.

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PP1

High-Dimensional Uncertainty Quantification of Fluid-Structure Interaction

This contribution discusses uncertainty quantification problems in fluid-structure interaction, using the pseudo-spectral approach, while focusing on high dimensional stochastic problems. Addressing the complexity posed by high dimensional uncertainty quantification is a challenging task, which is resolved using an approach comprising sparse grids interpolation and numerical quadrature. In post-processing, besides estimating the statistics, a Sobol's indices based sensitivity analysis is performed at no additional computational cost, using the already computed coefficients of the spectral expansion approximation.

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PP1

Algebraic Method for the Construction of a Series of Uniform Computer Designs

The incomplete block designs constructed from sub- spaces with mj dimension, $j = 1 , \ldots, k$ ($k < m$) of a projective geometry PG (m, pn) provide symmetric residual designs if $m_j = m-j$. Their union on the i^{th} step generates repeated resolvable designs. More economical designs are deducted. A judicious juxtaposition of these designs engenders n-ary designs and nested uniform Computer designs using the " RBIBD - UD" Algorithm.

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PP1

A Framework for Variational Data Assimilation with Superparameterization

Superparameterization (SP) is a multiscale computational approach wherein a large scale atmosphere or ocean model is coupled to an array of simulations of small scale dynamics on periodic domains embedded into the computational grid of the large scale model. SP has been successfully developed in global atmosphere and climate models, and is a promising approach for new applications, but there is currently no practical data assimilation framework that can be used with these models. The authors develop a 3D-Var variational data assimilation framework for use with SP; the relatively low cost and simplicity of 3D-Var in comparison with ensemble approaches makes it a natural fit for relatively expensive multiscale SP models. To demonstrate the assimilation framework in a simple model, the authors develop a new system of ordinary differential equations similar to the two-scale Lorenz-'96 model. The system has one set of variables denoted $\{Y_i\}$, with large and small scale parts, and the SP approximation to the system is straightforward. With the new assimilation framework the SP model approximates the large scale dynamics of the true system accurately.

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PP1

Identification of Aleatory Uncertainties in Material Properties

Recent works devoted to identification of aleatory uncertainties either assume known type of their probability distribution or model those uncertainties by polynomial chaos expansion. While the former approach leads to identification of (typically only few) statistical moments, the later one allows to identify more complex distributions defined by limited number of polynomial chaos coefficients. Here we aim to relax these assumptions and identify the distribution of aleatory uncertainties using Markov chain Monte Carlo method.

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PP1

Hybrid Reduced Basis Method and Generalized Polynomial Chaos for Stochastic Partial Differential Equations

The generalized Polynomial Chaos (gPC) method is a popular method for solving partial differential equations with random parameters. However, when the probability space has high dimensionality, the solution ensemble size required for an accurate gPC approximation can be large. We show that this process can be made more efficient by closely hybridizing gPC with Reduced Basis Methods (RBM). Furthermore, we demonstrate that this is achieved with essentially no loss of accuracy through numerical experiments.

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PP1

Using Training Realizations to Characterize, Identify, and Remove Model Errors in Bayesian Geophysical Inversion

MCMC sampling of the Bayesian posterior distribution is a growing means of performing UQ for geophysical problems. To improve computational tractability, simplified numerical models are often utilized, which can lead to strong posterior bias. With application to crosshole georadar tomography, we demonstrate how a suite of training realizations can be used to generate a sparse basis for known sources of model error, which can be used to identify and remove these errors in MCMC.

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PP1

Robust Experiment Design Based on Sobol Indices

Current advanced techniques for designing laboratory experiments use local sensitivities, which are merged into some optimality criterion further optimised by some robust optimisation algorithm. Use of local sensitivities, however, requires good prior guess of parameters to be identified

from the experiment, but such guess is typically no available. The aim of the presented contribution is to overcome this difficulty by introduction of global sensitivities based on Sobol indices.

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PP1

Π4U: An Hpc Framework for Bayesian Uncertainty Quantification of Large Scale Computational Models

Π4U is a task-parallel framework for non-intrusive Bayesian uncertainty quantification of computationally demanding physical models on massively parallel computing architectures. The framework incorporates asymptotic approximations and multiple sampling algorithms. Task-based parallelism is exploited with a platform-agnostic adaptive load balancing library that orchestrates scheduling of multiple physical model evaluations on computing platforms ranging from multicore systems to hybrid GPU clusters. Experimental results using representative applications demonstrate flexibility and excellent scalability of the proposed framework.

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PP1

Optimization of Expensive Black-Box Models Using Information Gain

Optimization often requires numerous evaluations of a quantity of interest through a potentially expensive model. To alleviate the cost of optimization, this work presents a strategy to adaptively construct and exploit a cheap surrogate for the optimization of expensive black-box models. This is achieved by defining a utility function that quantifies the information gained about the model in regions of interest. The next design to evaluate is chosen to maximize that utility function.

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PP1

Approximating Uncertain Dynamical Systems Using Time-Dependent Orthogonal Bases

We use time-dependent orthogonal bases (TDOB) to approximate stochastic dynamical systems. The object of this method is to track the stochastic response surface with quasi-optimal bases. The bases are adaptively modified so as to keep good approximation of stochastic response surfaces with time progresses. The bases are assumed to be orthonormal all the time. Under these assumptions, we derive the equations of motion for time-dependent orthogonal bases based on the variational principle.

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PP1

On Low-Rank Entropy Maximization of Covariance Matrices

We consider entropy maximization of covariance matrices regularized with nuclear norm. The motivation stems from applications where we seek low-dimensional stochastic inputs to linear systems given partial data on state covariance matrices. This inverse problem also arises from estimation of precision matrices in machine learning. We solve this constrained optimization problem via solving a sequence of linear equations. Based on a nullspace parameterization, we exploit special structure of Hessian matrices that makes matrix-vector multiplication efficient.

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PP1

Comparing Networks and Graphical Models at Different Scales

We consider the problem of local and global testing of dependent multiple hypotheses where dependency is represented by complex networks. By combining complex graph theory and statistical testing, we propose different kinds of tests that assess the deviance between data structure and null models or between groups of networks. We also show how to exploit data structure and prior information of dependency to derive hierarchical multiple testing procedures, without having to relying on strong assumptions.

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PP1

Sensitivity Analysis of the Uncertainty in Rapid Pressure Strain Correlation Models

We explicate upon the dynamics due to linear pressure in a variety of 2- and 3-dimensional mean flows. Our focus is to establish the import of the wave space (or dimensionality) information, and, to quantify the degree of the epistemic uncertainty due to its absence in the classical rapid pressure strain correlation models. We carry out sensitivity analysis to exhibit that the prediction intervals are highly dependent on the mean flow in consideration and to a lesser extent, upon the state of the Reynolds stress tensor. Such analysis and understanding is critical for formulating improved pressure strain correlation models.

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PP1

Uncertainty Classification for Strategic Energy Planning

Various countries and communities are defining strategic energy plans driven by concerns related to climate change and security of energy supply. The long time horizon inherent to strategic energy planning requires uncertainty to be accounted for. Uncertainty classification consists in defining the type of uncertainty involved and quantifying it. It is needed as input for uncertainty and sensitivity analyses, and optimization under uncertainty applications. In this work we define a methodology for uncertainty classification for a typical strategic energy planning problem. As an example, the methodology is applied to some representative parameters.

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PP1

Uncertainty Quantification in Large Civil Infrastructure

Replacing all aging civil infrastructure is not sustainable. Reserve capacity estimation of existing structures is typically performed through structural identification of various degrees of sophistication. In civil infrastructure, uncertainty is seldom Gaussian, often systematic and the correlation model is rarely known. An error-domain model-falsification methodology is presented with Markov-Chain Monte-Carlo sampling used for exploring solution spaces leading to robust identification and prediction for non-Gaussian and systematic uncertainty forms.

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PP1

Data Assimilation for Uncertainty Reduction in Forecasting Cholera Epidemics: An Application to the Haiti Outbreak

Spatially explicit models for the simulation of waterborne diseases must take into account uncertainties arising from the atmospheric forcing and epidemiological and environmental parameters. The real-time assimilation of the recorded infected cases is an indispensable requirement to reduce the uncertainties in the model forecast and, thus, make these tools operative in the management of an emergency. Here we show the efficacy of advanced DA schemes in improving the forecast of the Haiti cholera outbreak of 2010.

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PP1

State Dependent Model Error Characterization for Data Assimilation

Many existing methods for model error characterization in data assimilation focus only on estimating the first and second moments. We propose a framework to estimate the full distributional form based on model residuals. Conditional density estimation methods are used to develop the error distribution conditioned on model states for each assimilation time step. Errors in observations are simultaneously considered through deconvolution. Methods for transferring errors in observed variables to hidden states are also discussed.

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PP1

A Simple Alarm for Early Detection of Epidemics Over Networks

Forecasting the beginning of outbreaks of infectious diseases is well studied for the case of simple disease generating models. However, epidemics over real-world, heterogeneous networks tend to exhibit a more complex behavior. We propose a simple monitoring system suitable for non-homogeneous populations, and derive its statistical properties over simulated networks. We then illustrate its use on observed rates of influenza-like illness from the French Sentinelles network.

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PP1

Adaptive Optimal Designs for Dose-Finding Studies with Time-to-Event Outcomes on Continuous Dose Space

Many clinical trials use time-to-event outcomes as primary measures of efficacy or safety. In cancer trials the goals may be to estimate a dose-response relationship and a dose level that yields the longest progression-free survival for testing in subsequent studies. Finding efficient designs for such trials may be complicated due to uncertainty about the dose-response model, model parameters and censored observations. We develop optimal and adaptive designs for such trials.

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PP1

A New Algorithm for Sensor-Location Problems in the Sense of Optimal Design of Experiments for Pdes

We state an algorithm for the computation of a sparse optimal approximate design consisting of maximal $\frac{n(n+1)}{2}$ points (Dirac-Deltas) in an experimental domain Ω , based on a combined conditional and a proximal gradient method with an additional post-processing. The algorithm is able to add/remove sensors to/from multiple points in Ω and ensures that each iterate consists of max. $\frac{n(n+1)}{2}$ points. Weak*-Convergence of the iterates in the space of regular Borel measures is shown.

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PP1

A Fast Computational Method for Tracking the Evolving Spatial-Temporal Gene Networks Based on Topological Information

The modeling and identification of the spatial-temporal gene networks in transcriptome scale is a challenging problem. To investigate the molecular mechanisms of genes in a dynamic and systematic fashion, we develop a novel method for tracking the spatial-temporal modules of gene networks reconstructed from the brain development gene expression data. A fast computational method for topological graph matching is proposed to track the evolving gene networks. We apply this method to brain spatial-temporal networks and provide new insights into the molecular mechanisms of brain development as well as the functions of the schizophrenia-associated genes.

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PP1

Robust Optimization for Silicon Photonics Process Variations

Robust design under manufacturing process variations is critical in Electrical Engineering. The problem becomes intractable when dimensionality increases. In this work, we develop an efficient simulation technique to solve high dimensional robust optimization problems based on stochastic spectral methods and compressed sensing. The technique is applied to silicon photonic devices. Results show that the variance of the bandwidth in a coupled ring filter example is 31 % smaller when using our technique.

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PP1

Parameterization-Induced Model Discrepancy

Parameterization is a critical component of groundwater modeling because practitioners must balance computational burden with the need to express uncertainty in spatially-distributed properties and time-varying boundary conditions. Using FOSM theory, we have derived exact expressions for the penalty (e.g. increase in forecast uncertainty) for not casting uncertain model inputs as parameters; the penalty expresses the induced model discrepancy arising from parameter compensation. We show that choices made during the parameterization process can greatly affect the resulting forecast uncertainty.

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PP1

Efficient Gpce-Based Rock Characterization for the Analysis of a Hydrocarbon Reservoir

The contribution focuses on a gPCE based rock characterization inferring the parameters of a geomechanical model with seafloor surface measurements. The deformations are due to the pressure depletion within the subsurface rock formation caused by the extraction of gas from an offshore hydrocarbon reservoir. It is shown how the prior expert knowledge of the physical properties of the system is updated by incorporating the measurement data via Bayesian inference using surrogate model for the forward model. The reservoir characterization allows for predicting the propagation of further deformations and the long-term behaviour of the offshore platform.

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PP101

Active Subspaces: Theory and Practice

Active subspaces are an emerging set of tools for dimension reduction in parameter studies. This poster will outline the essential elements of the theory and practice of active subspaces.

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PP101

Active Subspaces: Deriving Metrics for Sensitivity Analysis

Active subspaces are an emerging set of tools for parameter studies. Sensitivity analysis helps us understand output variation corresponding to parameters of a model. We propose two new sensitivity metrics constructed from active subspaces and relate them to existing global sensitivity metrics such as the Sobol' Index and derivative-based sensitivity metrics. In addition, we analyze two mathematical models to compare results of each metric.

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PP101

Active Subspaces: Quantifying Errors in Surrogate Models of Failure Probability

Application of active subspaces to aid in estimation of probabilities of rare events.

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PP101

Active Subspaces: Application to Gas Turbine Design and Optimization

Application of the active subspace dimensionality reduction methods to approximate complex gas turbine airfoil design spaces to motivate optimization and stochastic solutions.

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PP101

Active Subspaces: Hypercube Domains and Zonotopes

Motivated by applications of Active Subspaces to integration on a hypercube domain in high dimension, we detail a probabilistic algorithm for enumerating vertices of a zonotope.

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PP102

MUQ (MIT Uncertainty Quantification): Algorithms and Interfaces for Solving Forward and Inverse Uncertainty Quantification Problems

Standard forward and inverse uncertainty quantification algorithms, such as polynomial chaos and Markov chain Monte Carlo, share many common building blocks. We describe how the MIT Uncertainty Quantification (MUQ) library implements these building blocks and how our implementation leads to extensible and easy-to-use software. In particular, we illustrate MUQ's user interfaces for defining new algorithms and implementing new models, and how appropriate software abstractions are used to create these interfaces.

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PP102

UQ with the Spatially Adaptive Sparse Grid Toolkit SG++

SG++ is a multi-platform toolkit that excels by fast and efficient algorithms for spatially adaptive sparse grids. 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 and Sobol-indices for sensitivity analysis, or the Rosenblatt transformation for estimated sparse grid densities. We show use cases and its convenient use via its rich interfaces to Python and Matlab.

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PP102

Practical Use of Chaospy for Pedestrian Traffic Simulations

We applied chaospy for forward UQ simulations of pedestrian evacuation scenarios. Chaospy proved to be very flexible and extensible when coupled to a black-box solver. Additional functionality concerning pre-/postprocessing of data as well as the parallel execution of the traffic simulations on a cluster can easily be realised in python directly. The poster shows the whole simulation pipeline, from the setup to the visualisation of the uncertainty, which the application scientists can easily interpret.

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PP102

Implementation of UQ Workflows with the C++/Python UQTk Toolkit

The UQ Toolkit (UQTk) is a collection of libraries, tools and apps for uncertainty quantification in computational models. UQTk offers intrusive and non-intrusive methods for forward uncertainty propagation and sensitivity analysis, as well as inverse modeling via Bayesian inference. The Python interface allows easy prototyping and developing common UQ workflows that rely on C++ libraries. The poster will demonstrate details of such workflows to highlight key UQTk capabilities in practical settings.

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PP102

Dakota: Algorithms for Design Exploration and Simulation Credibility

The Dakota toolkit provides a flexible interface between simulations and iterative analysis methods including optimization, uncertainty quantification, parameter estimation, and sensitivity analysis. Methods may be used individually or as components within advanced strategies to address questions like "What is the best design?", "How safe is it?", and "How much confidence do I have in my answer?". We present a use case to illustrate how Dakota informs engineering decisions, highlighting emerging activity-based support mechanisms intended to facilitate non-expert use.

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PP102

Uqlab: a General-Purpose Matlab-Based Platform for Uncertainty Quantification

The UQLab project, developed at the Chair of Risk, Safety and Uncertainty Quantification at ETH Zurich, offers a modular MATLAB-based software framework that enables both industrial and academic users to easily deploy and develop advanced uncertainty quantification algorithms. Its flexible, black-box-oriented and easy-to-extend modular design is aimed at scientists without extensive IT background. This contribution gives a general overview of the current platform capabilities.

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PP102

Cossan-X: General Purpose Software for Uncertainty Quantification and Risk Management

COSSAN-X is a software package developed to make the concepts and technologies of uncertainty quantification and risk analysis available for anyone to use. COSSAN-X is a general-purpose software tool that can be used to solve a wide range of engineering and scientific problems (e.g. uncertainty quantification, reliability analysis, sensitivity optimisation, robust design and life-cycle management). The software package is based on the most recent and advanced algorithms for the rational quantification and propagation of uncertainties. Its modular structure also allows for the easy extension and implementation of new toolkits.

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