Advances in Uncertainty Quantification Methods, Algorithms and Applications (UQAW 2014)

January 6 -10, 2014
9:00 a.m. to 5:00 p.m.
Level 0 auditorium, between Al-Jazri and Al-Kindi
(buildings 4 and 5)

WORKSHOP TOPICS

- Uncertainty Quantification Methods and Algorithms
- Verification and Validation
- Application to Problems in Computational Science and Engineering, Networks, and the Environment

ORGANIZERS

- **Raul Tempone,** Computer, Electrical, and Mathematical Sciences and Engineering Division, KAUST
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Sponsored by SRI – Center for Uncertainty Quantification

Welcome from the Directors of KAUST SRI Center for Uncertainty Quantification in Computational Science and Engineering

On Behalf of SRI Center for Uncertainty Quantification in Computational Science and Engineering, we are delighted to welcome you to KAUST, and to 2nd annual meeting of the Center, *Advances in Uncertainty Quantification Methods, Algorithms and Applications* (UQAW2014), January 6-10, 2014 at KAUST in Thuwal, KSA.

First and foremost, we wish to thank the Advisory Board members who have accepted to join us for this meeting, along with all the attendees, and of course of the Thrust Leaders and the team members.

This second annual meeting is intended to report on the latest advances and innovations in Uncertainty Quantification Methods, Algorithms and Applications (UQAW 2014); as well as serve as a discussion forum for exchanging information about the development, application, and experimental results by bringing together researchers, academics, and students working in the field.

It is with great pleasure that we present these proceedings of abstracts and posters. The annual meeting is very successful with over 72 contributions (as oral or poster presentations) together with 23 invited talks delivered from authors of the Center and from diverse international affiliations (e.g. United States, Germany, Canada, France, Greece, UK, and others). By organizing UQAW 2014, it is our sincere hope to help promote and broaden the diffusion of the research activities in the Uncertainty Quantification field.

We would like to express our sincere appreciation to the staff and to colleagues who participate in the workshop.

KAUST, November 2013 *Raúl Tempone and Omar Knio*

Organization Committee

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	Mon Jan 6	Tue Jan 7	Wed Jan 8	Thur Jan 9	Fri Jan 10
8:30 9:00	Breakfast	Breakfast	Breakfast	Breakfast	Local Meetings
9:00 9:30	Welcome Registration	Center Presentation for Board Members Reserved to at KAUST and external participants of SRI-UQ Center	external talk 5 : Quasi-Monte Carlo FE Methods for Elliptic PDEs with Log-normal Random Coefficients **Robert Scheichl**	center talk 10: Dimension-independent, likelihood informed sampling for Bayesian inverse problems **Kody Law**	
9:30 10:00	center talk 1: A Highly Stable Marching-on-in-Time Volume Integral Equation Solver **Hakan Bagci**		external talk 6: Analyzing rare events with Monte Carlo: advanced methods **Gerardo Rubino**	external talk 9: Multivariate max-stable spatial processes **Marc Genton**	
10:00 10:30	center talk 2: Optimal Design of Shock Tube Experiments for Parameter Inference **Omar Knio**		center talk 9: Physical Layer Security **Zouheir Rezki**	external talk 10: Convergence of multilevel sample variance estimators: random obstacle problems **Alexey Chernov**	
10:30 11:00	Break	Break	Break	Break	
11:00 11:30	external talk 1: Collocation methods for UQ in PDE models with random data **Fabio Nobile**	center talk 6: On the Predictability of Computer simulations **Serge Prudhomme**	external talk 7: Kernel methods for UQ **Christian Rieger**	center talk 11: time dependent mean field games **Diogo Gomes**	
11:30 12:00	external talk 2: Cooperative HARQ with Poisson Interference and Opportunistic Routing **Mostafa Kaveh**	center talk 7: Spectral methods for UQ in the incompressible Navier-Stokes equations **Olivier Le Maitre**	external talk 8: Numerical Methods for Bayesian Inverse Problems **Oliver Ernst**	external talk 11: An adaptive Drift Implicit Euler method for SDEs **Georgios Zouraris**	
12:00 13:30	Lunch	Lunch	Lunch	Lunch	Lunch
13:30 14:00	center talk 3: Channel capacity computation in generalized fading environments **Slim Alouini**	Advisory Board Meeting	Advisory Board Meeting Followup	Advisory Board Report Presentation	Local Activities
14:00 14:30	center talk 4: Cooperative Games for Smarter Cities **Tembine Hamidou**				
14:30 15:00	Break				
15:00 15:30	external talk 3: Model reduction and synthesis for UQ **Roger Ghanem**	Board Members Discussion	Board Members Discussion	Social activity: Economic City Beach	
15:30 16:00	center talk 5: Inverse problems and UQ **Alexander Litvinenko**	external talk 4: Optimal Experimental Design for Large-Scale Bayesian Inverse Problems **Omar Ghattas**	Poster Session		
16:00 16:30	Poster set-up	center talk 8: Size Estimates in Inverse Problems **Michele Di Cristo**			
16:30 17:00					
	Welcome Reception: Campus Library	Thuwal Dinner: Fish Restaurant	Conference Dinner: Yacht Club	Economic City Dinner	

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Oral presentations

A Highly Stable Marching-on-in-Time Volume Integral Equation Solver for Analyzing Transient Wave Interactions on High-Contrast Scatterers

Hakan Bagci

Time domain integral equation (TDIE) solvers represent an attractive alternative to finite difference (FDTD) and finite element (FEM) schemes for analyzing transient electromagnetic interactions on composite scatterers. Current induced on a scatterer, in response to a transient incident field, generates a scattered field. First, the scattered field is expressed as a spatio-temporal convolution of the current and the Green function of the background medium. Then, a TDIE is obtained by enforcing boundary conditions and/or fundamental field relations. TDIEs are often solved for the unknown current using marching on-in-time (MOT) schemes. MOT-TDIE solvers expand the current using local spatio-temporal basis functions. Inserting this expansion into the TDIE and testing the resulting equation in space and time yields a lower triangular system of equations (termed MOT system), which can be solved by marching in time for the coefficients of the current expansion. Stability of the MOT scheme often depends on how accurately the spatio-temporal convolution of the current and the Green function is discretized. In this work, band-limited prolate-based interpolation functions are used as temporal bases in expanding the current and discretizing the spatio-temporal convolution. Unfortunately, these functions are two sided, i.e., they require "future" current samples for interpolation, resulting in a non-causal MOT system. To alleviate the effect of non-causality and restore the ability to march in time, an extrapolation scheme can be used to estimate the future values of the currents from their past values. Here, an accurate, stable and band-limited extrapolation scheme is developed for this purpose. This extrapolation scheme uses complex exponents, rather than commonly used harmonics, so that propagating and decaying mode fields inside the dielectric scatterers are accurately modeled. The resulting MOT scheme is applied to solving the time domain volume integral equation (VIE). Numerical results demonstrate that this new MOT-VIE solver maintains its stability and accuracy even when used in analyzing transient wave interactions on high-contrast scatterers.

King Abdullah University of Science and Technology, Saudi Arabia

Optimal Design of Shock Tube Experiments for Parameter Inference

Omar Knio

We develop a Bayesian framework for the optimal experimental design of the shock tube experiments which are being carried out at the KAUST Clean Combustion Research Center. The unknown parameters are the pre-exponential parameters and the activation energies in the reaction rate expressions. The control parameters are the initial mixture composition and the temperature. The approach is based on first building a polynomial based surrogate model for the observables relevant to the shock tube experiments. Based on these surrogates, a novel MAP based approach is used to estimate the expected information gain in the proposed experiments, and to select the best experimental set-ups yielding the optimal expected information gains. The validity of the approach is tested using synthetic data generated by sampling the PC surrogate. We finally outline a methodology for validation using actual laboratory experiments, and extending experimental design methodology to the cases where the control parameters are noisy.

KAUST

Collocation methods for uncertainty quantification in PDE models with random data

Fabio Nobile

In this talk we consider Partial Differential Equations (PDEs) whose input data are modeled as random fields to account for their intrinsic variability or our lack of knowledge.

After parametrizing the input random fields by finitely many independent random variables, we exploit the high regularity of the solution of the PDE as a function of the input random variables and consider sparse polynomial approximations in probability (Polynomial Chaos expansion) by collocation methods.

We first address interpolatory approximations where the PDE is solved on a sparse grid of Gauss points in the probability space and the solutions thus obtained interpolated by multivariate polynomials. We present recent results on optimized sparse grids in which the selection of points is based on a knapsack approach and relies on sharp estimates of the decay of the coefficients of the polynomial chaos expansion of the solution.

Secondly, we consider regression approaches where the PDE is evaluated on randomly chosen points in the probability space and a polynomial approximation constructed by the least square method. We present recent theoretical results on the stability and optimality of the approximation under suitable conditions between the number of sampling points and the dimension of the polynomial space. In particular, we show that for uniform random variables, the number of sampling point has to scale quadratically with the dimension of the polynomial space to maintain the stability and optimality of the approximation. Numerical results show that such condition is sharp in the monovariate case but seems to be over-constraining in higher dimensions. The regression technique seems therefore to be attractive in higher dimensions.

Scientific Computing and Uncertainty Quantification, Ecole Polytechnique Federale de Lausanne, Switzerland

Cooperative HARQ with Poisson Interference and Opportunistic Routing

Amogh Rajana and Mostafa Kaveh

This presentation considers reliable transmission of data from a source to a destination, aided cooperatively by wireless relays selected opportunistically and utilizing hybrid forward error correction/detection, and automatic repeat request (Hybrid ARQ, or HARQ). Specifically, we present a performance analysis of the cooperative HARQ protocol in a wireless adhoc multihop network employing spatial ALOHA. We model the nodes in such a network by a homogeneous 2-D Poisson point process. We study the tradeoff between the per-hop rate, spatial density and range of transmissions inherent in the network by optimizing the transport capacity with respect to the network design parameters, HARQ coding rate and medium access probability. We obtain an approximate analytic expression for the expected progress of opportunistic routing and optimize the capacity approximation by convex optimization. By way of numerical results, we show that the network design parameters obtained by optimizing the analytic approximation of transport capacity closely follows that of Monte Carlo based exact transport capacity optimization. As a result of the analysis, we argue that the optimal HARQ coding rate and medium access probability are independent of the node density in the network.

Department of Electrical and Computer Engineering University of Minnesota Minneapolis, Minnesota, USA

On the computation of the channel capacity in generalized fading environments

Mohamed-Slim Alouini

Exact and asymptotic studies of the average error probability of wireless communication systems over generalized fading channels have been extensively pursued over the last two decades. In contrast, studies and results dealing with the channel capacity in these environments have been more scarce. In the first part of this talk, we present a generic moment generating function-based approach for the exact computation of the channel capacity in such kind of environments. The resulting formulas are applicable to systems having channel state information (CSI) at the receiver and employing maximal-ratio combining or equal-gain combining multichannel reception. The analysis covers the case where the combined paths are not necessarily independent or identically distributed. In all cases, the proposed approach leads to an expression of the ergodic capacity involving a single finite-range integral, which can be easily computed numerically. In the second part of the talk, we focus on the asymptotic analysis of the capacity in the high and low signal-to-noise ratio (SNR) regimes. More specifically, we offer new simple closed-form formulas that give an intuitive understanding of the capacity behavior at these two extreme regimes. Our characterization covers not only the case where the CSI is available only at the receiver but also the case where the CSI is available at both the transmitter and receiver.

King Abdullah University of Science and Technology, Saudi Arabia

Cooperative Mean-Field Type Games for Smarter Cities

Hamidou Tembine

In the standard formulation of a game, a player's payoff function depends on the states and actions of all the players. Yet, real world applications suggest to consider also a functional of the probability measure of states and actions of all the players. In this talk, we focus on cooperative mean-field type games in which the state dynamics and the payoffs depend not only on the state and action profiles but also on a functional of their probability measure. We establish a stochastic maximum principle (SMP) and provide a time-dependent payoff allocation procedure for coalitions. The allocated payoff considers not only a fairness property but also the cost of making the coalition. In order to understand the sustainability of cooperation in the long term, time consistency and subgame perfectness solution concept equations are established. We then establish a risk-sensitive SMP for exponential-integral payoff functional of mean-field type. The methodology is applied to smart cities where the city pollution by agricultural and industry activities and the viability of the ecosystem need to be carefully designed.
This is a joint long-run collaborative work with Tamer Basar (Illinois), Dario Bauso (Palermo University), Ben Mansour Dia (KAUST), Boualem Djehiche (KTH), Raul Tempone (KAUST), Quanyan Zhu (New York University).

KAUST SRI Center for Uncertainty Quantification in Computational Science and Engineering, King Abdullah University of Science and Technology, Saudi Arabia

Model reduction and synthesis for UQ

Roger Ghanem

We describe model reduction adapted to the polynomial chaos approach for characterizing and propagation uncertainty in physics-based models. In such circumstances model reduction will generally pertain to a reduction with respect to both uncertainty and physics. Standard approaches to uncertainty analysis are generally limited in their ability at UQ reduction to moment truncation. Polynomial chaos constructions, on the other hand, have access to a full complement of mathematical structure, such as projections and best approximations.

We describe procedures for model reduction of uncertainty systems that capitalize on these Polynomial chaos constructions. Specifically, we describe a recent approach, and demonstrate its significance to problems involving multiscale and multiphysics interactions. This approach focuses on a particular quantity of interest (QoI) and recognizes that in several important cases, these QoI are low-dimensional. We describe classes of problems where reduction to one-dimensional approximations yield very good approximations to the original high-dimensional problem. The significance of these algorithms on applications is transformative as they enable the resolution of problems that could otherwise be deemed prohibitive.

Inverse problems and uncertainty quantification

Alexander Litvinenko and Hermann G. Matthies

In a Bayesian setting, inverse problems and uncertainty quantification (UQ) - the propagation of uncertainty through a computational (forward) modelare strongly connected. In the form of conditional expectation the Bayesian update becomes computationally attractive. This is especially the case as together with a functional or spectral approach for the forward UQ there is no need for time- consuming and slowly convergent Monte Carlo sampling. The developed sampling- free non-linear Bayesian update is derived from the variational problem associated with conditional expectation. This formulation in general calls for further discretisa- tion to make the computation possible, and we choose a polynomial approximation. After giving details on the actual computation in the framework of functional or spectral approximations, we demonstrate the workings of the algorithm on a number of examples of increasing complexity. At last, we compare the linear and quadratic Bayesian update on the small but taxing example of the chaotic Lorenz 84 model, where we experiment with the influence of different observation or measurement operators on the update.

KAUST SRI UQ Center and Institute of Scientific Computing, Technische Universitaet Braunschweig

On the Predictability of Computer simulations: Advances in Verification and Validation

Serge Prudhomme

We will present recent advances on the topics of Verification and Validation in order to assess the reliability and predictability of computer simulations. The first part of the talk will focus on goal-oriented error estimation for nonlinear boundary-value problems and nonlinear quantities of interest, in which case the error representation consists of two contributions: 1) a first contribution, involving the residual and the solution of the linearized adjoint problem, which quantifies the discretization or modeling error; and 2) a second contribution, combining higher-order terms that describe the linearization error. The linearization error contribution is in general neglected with respect to the discretization or modeling error. However, when nonlinear effects are significant, it is unclear whether ignoring linearization effects may produce poor convergence of the adaptive process. The objective will be to show how both contributions can be estimated and employed in an adaptive scheme that simultaneously controls the two errors in a balanced manner. In the second part of the talk, we will present a novel approach for calibration of model parameters. The proposed inverse problem not only involves the minimization of the misfit between experimental observables and their theoretical estimates, but also an objective function that takes into account some design goals on specific design scenarios. The method can be viewed as a regularization approach of the inverse problem, one, however, that best respects some design goals for which mathematical models are intended. The inverse problem is solved by a Bayesian method to account for uncertainties in the data. We will show that it shares the same structure as the deterministic problem that one would obtain by multi-objective optimization theory. The method is illustrated on an example of heat transfer in a two-dimensional fin. The proposed approach has the main benefit that it increases the confidence in predictive capabilities of mathematical models.

Department of Mathematics and Industrial Engineering, Ecole Polytechnique de Montréal, Canada

Recent advances in spectral methods for parametric uncertainty propagation in the incompressible Navier-Stokes equations

Olivier Le Maître

In this talk, I will present two recent contributions to the development of efficient methodologies for uncertainty propagation in the incompressible Navier-Stokes equations. The first one concerns the reduced basis approximation of stochastic steady solutions, using Proper Generalized Decompositions (PGD). An Arnoldi scheme is introduced to construct a reduced basis of deterministic velocity functions onto which the stochastic problem is projected to obtain a low dimensional Galerkin problem. The construction then amounts to the resolution of a sequence of uncoupled deterministic Navier-Stokes like problem and simple quadratic stochastic problems, followed by the resolution of a low-dimensional coupled quadratic stochastic problem, with a resulting complexity which has to be contrasted with the dimension of the whole Galerkin problem for classical spectral approaches. An efficient algorithm for the approximation of the stochastic pressure field is also proposed. Computations are presented for uncertain viscosity and forcing term to demonstrate the effectiveness of the reduced method. The second contribution concerns the computation of stochastic periodic solutions to the Navier-Stokes equations. The objective is to circumvent the well-known limitation of spectral methods for long-time integration. We propose to directly determine the stochastic limit-cycles through the definition of its stochastic period and an initial condition over the cycle. A modified Newton method is constructed to compute iteratively both the period and initial conditions. Owing to the periodic character of the solution, and by introducing an appropriate time-scaling, the solution can be approximated using low-degree polynomial expansions with large computational saving as a result. The methodology is illustrated for the von-Karman flow around a cylinder with stochastic inflow conditions.

National Center for Scientific Research (CNRS), LIMSI-Lab, Orsay, France

Optimal Experimental Design for Large-Scale Bayesian Inverse Problems

Omar Ghattas, Alen Alexanderian, Noemi Petra, and Georg Stadler

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 find optimal sensor locations that minimize the average variance of a Gaussian approximation of the posterior parameter probability distribution at the maximum a posterior (MAP) point. The OED problem is thus an infinite dimensional optimization problem with the trace of the inverse Hessian operator at the MAP point as is objective functional, and constraints composed of the necessary conditions defining the MAP point solution of the inverse problem (forward, adjoint, and gradient PDEs) as well as PDEs defining the action of the inverse Hessian (incremental forward, incremental adjoint, and inverse Hessian action). The optimization variables are weights associated with predefined sensor locations. These weights are sparsified with L1 or L0 regularization terms. Numerical results are presented for the problem of determining optimal sensor locations associated with inference of the permeability field in a porous medium flow problem. The results indicate that the cost of finding the optimal sensor locations, measured in terms of forward PDE solves, scales independently of the state variable dimension, the parameter dimension, and the data/sensor dimension.

The University of Texas at Austin

Size Estimates in Inverse Problems

Michele Di Cristo

Detection of inclusions or obstacles inside a body by boundary measurements is an inverse problems very useful in practical applications. When only finite numbers of measurements are available, we try to detect some information on the embedded object such as its size. In this talk we review some recent results on several inverse problems. The idea is to provide constructive upper and lower estimates of the area/volume of the unknown defect in terms of a quantity related to the work that can be expressed with the available boundary data.

Quasi-Monte Carlo FE Methods for Elliptic PDEs with Log-normal Random Coefficients

I.G. Graham, F.Y. Kuo, J.A. Nicholls, R. Scheichl, Ch. Schwab and I.H. Sloan

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

University of Bath

Analyzing rare events with Monte Carlo: advanced methods

Gerardo Rubino

When systems are complex and critical, and when we are interested in their dependability properties (reliability, availability in its many forms, etc.), only simulation can be used for their analysis: if the system is complex, analytical and numerical procedures are in general useless. In this situation, the main difficulty relies in the rare event problem: if the system is critical, catastrophic failures have small probabilities to occur (but huge consequences, making their study critical as well). In this talk we briefly describe the two main families of Monte Carlo techniques that are used today in the area: Importance Sampling and the specific Zero-Variance approach, and Splitting procedures. Some examples will illustrate the presentation.

INRIA, France

Physical Layer Security

Zouheir Rezki

Kernel methods for uncertainty quantification

Michael Griebel, Christian Rieger and Barbara Zwicknagl

The modeling of uncertainties in differential equations naturally leads to high dimensional reconstruction problems. Without exploiting further information, those problems are numerically unfeasible. In this talk, we show how the regularity theory for parametric partial differential equations leads to reproducing kernel Hilbert spaces. This motivates the use of (kernel–based) mesh-less reconstruction methods which reflect the parametric regularity. Furthermore, there are additional dimension reduction techniques, typically from machine learning, available for kernel–based methods. We demonstrate how so–called sampling inequalities can be employed to derive a priori deterministic error estimates for some of the regularized algorithms from machine learning. These error estimates allow to identify the influence of certain regularization parameters and hence lead to a priori parameter choices.

University of Bonn

Numerical Methods for Bayesian Inverse Problems

Oliver G. Ernst, Björn Sprungk, K. Andrew Cliffe, Hans-Jörg Starkloff

We present recent results on Bayesian inversion for a groundwater flow problem with an uncertain conductivity field. In particular, we show how direct and indirect measurements can be used to obtain a stochastic model for the unknown. The main tool here is Bayes' theorem which merges the indirect data with the stochastic prior model for the conductivity field obtained by the direct measurements. Further, we demonstrate how the resulting posterior distribution of the quantity of interest, in this case travel times of radionuclide contaminants, can be obtained by Markov Chain Monte Carlo (MCMC) simulations. Moreover, we investigate new, promising MCMC methods which exploit geometrical features of the posterior and which are suited to infinite dimensions.

Oliver G. Ernst
TU Chemnitz, Department of Mathematics and Björn Sprungk
TU Chemnitz, Department of Mathematics, K. Andrew Cliffe
University of Nottingham, School of Mathematical Sciences and Hans-Jörg Starkloff
University of Applied Sciences Zwickau, Fachgruppe Mathematik

Dimension-independent, likelihood informed sampling for Bayesian inverse problems

Kody Law, Tiangang Cui, and Youssef Marzouk

When cast in a Bayesian setting, the solution to an inverse problem is given as a distribution over the space where the quantity of interest lives. When the quantity of interest is in principle a field then the discretization is very high dimensional. Formulating algorithms which are defined in the infinite-dimensional function space yields dimension-independent algorithms, which overcome the so-called curse of dimensionality. These algorithms may still be too expensive to implement in practical time-sensitive applications but can still be effectively used offline and on toy-models in order to benchmark the ability of more tractable approximate alternatives to quantify uncertainty in very high-dimensional problems. Furthermore, such limitations on the use of these algorithms are dictated by the current petascale computing environment and once we transition to exascale computing it will become feasible to use such algorithms in practical online applications. Inspired by the recent development of pCN and other function-space samplers [1], and also the recent independent development of Riemann manifold methods [2] and stochastic Newton methods [3], we propose a class of proposals [4,5] for Metropolis-Hastings algorithms which combine the benefits of both, yielding various dimension-independent and likelihood-informed (DILI) sampling algorithms. These algorithms can be effective at sampling from very high-dimensional posterior distributions.

References:

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2. M. Girolami, B. Calderhead. ”Riemann manifold Langevin and Hamiltonian Monte Carlo methods,” Journal of the Royal Statistical Society: Series B (Statistical Methodology) 73 (2), 123214 (2011).
3. J. Martin, L. Wilcox, C. Burstedde, O. Ghattas. ”A stochastic newton mcmc method for large-scale statistical inverse problems with application to seismic inversion,” SIAM Journal on Scientific Computing 34(3), 14601487 (2012).
4. K. J. H. Law. ”Proposals Which Speed Up Function-Space MCMC,” Journal of Computational and Applied Mathematics, in press (2013). http://dx.doi.org/10.1016/j.cam.2013.07.026
5. T. Cui, K.J.H. Law, Y. Marzouk. Dimension-independent, likelihood- informed samplers for Bayesian inverse problems. In preparation.

KAUST and MIT

Multivariate max-stable spatial processes

Marc G. Genton

Analysis of spatial extremes is currently based on univariate processes. Max-stable processes allow the spatial dependence of extremes to be modelled and explicitly quantified, they are therefore widely adopted in applications. For a better understanding of extreme events of real processes, such as environmental phenomena, it may be useful to study several spatial variables simultaneously. To this end, we extend some theoretical results and applications of max-stable processes to the multivariate setting to analyze extreme events of several variables observed across space. In particular, we study the maxima of independent replicates of multivariate processes, both in the Gaussian and Student-t cases. Then, we define a Poisson process construction in the multivariate setting and introduce multivariate versions of the Smith Gaussian extremevalue, the Schlather extremal-Gaussian and extremal-t, and the BrownResnick models. Inferential aspects of those models based on composite likelihoods are developed. We present results of various Monte Carlo simulations and of an application to a dataset of summer daily temperature maxima and minima in Oklahoma, U.S.A., highlighting the utility of working with multivariate models in contrast to the univariate case. Based on joint work with Simone Padoan and Huiyan Sang.

KAUST

Convergence of multilevel sample variance estimators and application for random obstacle problems

Alexey Chernov, Claudio Bierig

The Multilevel Monte Carlo Method (MLMC) is a recently established sampling approach for uncertainty propagation for problems with random parameters. In this talk we present new convergence theorems for the multilevel variance estimators. As a result, we prove that under certain assumptions on the parameters, the variance can be estimated at essentially the same cost as the mean, and consequently as the cost required for solution of one forward problem for a fixed deterministic set of parameters. We comment on fast and stable evaluation of the estimators suitable for parallel large scale computations. The suggested approach is applied to a class of scalar random obstacle problems, a prototype of contact between deformable bodies. In particular, we are interested in rough random obstacles modelling contact between car tires and variable road surfaces. Numerical experiments support and complete the theoretical analysis.

Department of Mathematics and Statistics, University of Reading

On time dependent mean-field games

D. Gomes, E. Pimentel, H. Sanchez-Morgado

In this talk we will report on new results concerning the existence of smooth solutions for time dependent mean-field games. This new result is established through a combination of various tools including several a-priori estimates for time-dependent mean-field games combined with new techniques for the regularity of Hamilton-Jacobi equations.

An adaptive Drift Implicit Euler method for SDEs

Georgios Zouraris

We propose a general framework to construct adaptive methods for the weak approximation problem of Ito stochastic differential equations, which we apply on variances of the Drift Implicit Euler method.
Joint work with Ernesto Mordecki (Universidad de la Republica, Montevideo, Uruguay), Anders Szepessy (KTH, Stockholm, Sweden), Raul Tempone (KAUST, Thuwal, KSA)

Department of Mathematics, University of Crete

Poster session I

Sampling methods

I-1

Strong Adaptive Multi-Level Monte Carlo

Håkon Hoel, Juho Happola and Raúl Tempone

We present a multilevel Monte Carlo (MLMC) method for weak approximation of stochastic differential equations (SDE) for which SDE realizations on all levels are generated using an a posteriori adaptive Euler–Maruyama step-size control for the strong error. Strong error adaptivity turns out to be useful for weak approximation MLMC methods since controlling the strong error of realizations at all levels provides a reliable and efficient way to control the statistical error of the weak approximation MLMC estimator. For a large set of low-regularity weak approximation problems the developed adaptive method produces output whose weak error is bounded by $\mathcal{O}(\varepsilon)$ at the cost $\mathcal{O}(\varepsilon^{-2}|\log(\varepsilon)|^3)$, which is a lower asymptotic cost than typically can be obtained by the uniform time-step MLMC method on the problems studied. Furthermore, numerical studies are provided for 1D and higher dimensional low-regularity weak approximation problems where the adaptive MLMC method outperforms the uniform time-step MLMC method in terms of computer runtime.

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I-2

Pore-scale uncertainty quantification with multilevel Monte Carlo

Matteo Icardi, Håkon Hoel, Quan Long, Raúl Tempone

Computational fluid dynamics simulations of pore-scale transport processes in porous media have recently gained popularity to understand complex physical processes, such as groundwater remediation and carbon sequestration, and derive effective equations and parameters for macro-scale reservoir simulation. However the geometrical details of the pore structures can be known only in a very low number of samples thanks to expensive micro-tomographic data and extraction operations. Furthermore, due to the computational complexity, the detailed flow computations can be carried out only on a limited number of cases and samples. Therefore the estimation of intrinsic uncertainty on the results, caused by the random sampling of the geometry and the one introduced by boundary conditions and uncertain flow parameters, is an important issue to analyze and it is often overlooked in the classical pore-scale approaches where equations are solved only in a deterministic context. The explicit introduction of randomness in the geometry and in other setup parameters can instead be crucial for the design and optimization of the number of pore-scale samples and simulations in real macro-scale problems. Recently developed uncertainty quantification tools, such as sparse polynomial chaos approximation, can be applied to study the variability in the output quantities of interests minimizing the number of computational samples. In our case, since there are no generic way to parametrize the randomness in the pore-scale structures, Monte Carlo techniques are the most accessible to compute statistics on random pore-scale geometries. To overcome the prohibitive computational cost of the standard Monte Carlo, we propose a multilevel Monte Carlo technique to reduce the computational cost of estimating quantities of interest within a prescribed accuracy constraint. Random samples of pore geometries and setup parameters, with a hierarchy of geometrical complexities and grid refinements, are synthetically generated and used to propagate the uncertainties in the simulation of single- and multi-phase flow simulations and compute statistics of the desired quantities of interest.

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I-3

On non-asymptotic optimal stopping criteria in Monte Carlo simulations

Christian Bayer, Håkon Hoel, Erik von Schwerin, Raúl Tempone

Consider the setting of estimating the mean of a random variable by a sequential stopping rule Monte Carlo (MC) method. Given the requirement that the estimate error should be smaller than a given tolerance $\mathrm{TOL} > 0$, how do you decide when to stop increasing the number of samples in your sequential MC method? An appeal to the central limit theorem leads to the typical second moment based sequential stopping rule MC which generally tends to perform well in the asymptotic regime when $\mathrm{TOL} \to 0$. This poster will show examples where such a stopping rule is unreliable in the non-asymptotic regime and present a higher moment based stopping rule which is shown in numerical examples to perform more reliably and only slightly less efficiently than the second moment based stopping rule. The work presented in this poster is available as a preprint [1].

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I-4

Multi Level Monte Carlo methods with Control Variate for elliptic SPDEs

Fabio Nobile, Erik von Schwerin, Raúl Tempone and Francesco Tesei

We consider the numerical approximation of the stochastic Darcy problem and propose to use a Multilevel Monte Carlo approach combined with a control variate variance reduction technique on each level. The control variate is obtained starting from the solution of an auxiliary regularized problem and its expected value is computed with a Stochastic Collocation method on the finest level in which it appears. Numerical examples and a comparison with the standard MLMC method are also presented.

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I-5

Hybrid Chernoff Tau-Leap

Alvaro Moraes, Raúl Tempone and Pedro Vilanova

Markovian pure jump processes model a wide range of phenomena, including chemical reactions at the molecular level, dynamics of wireless communication networks and the spread of epidemic diseases in small populations. There exist algorithms like Gillespie's SSA or Anderson's Modified Next Reaction Method, that simulates a single trajectory with the exact distribution of the process, but this can be time consuming when many reactions take place during a short time interval. Gillespie's approximated tau-leap method, on the other hand, can be used to reduce computational time, but it may lead to non-physical values due to a positive one-step exit probability, and it also introduces a time discretization error. Here, we present a novel hybrid algorithm for simulating individual trajectories which adaptively switches between the SSA and the tau-leap method. The switching strategy is based on a comparison of the expected inter-arrival time of the SSA and an adaptive time step derived from a Chernoff-type bound for the one-step exit probability. Because this bound is non-asymptotic, we do not need to make any distributional approximation for the tau-leap increments. This hybrid method allows us (i) to control the global exit probability of any simulated trajectory, and (ii) to obtain accurate and computable estimates of the expected value of any smooth observable of the process with minimal computational work. We present numerical examples that illustrate the performance of the proposed method.

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I-6

Multilevel Hybrid Chernoff Tau-Leap

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In this work, we extend the hybrid Chernoff tau-leap method to the multilevel Monte Carlo setting. Inspired by the work of Anderson and Higham on 2012 on tau-leap multilevel Monte Carlo with uniform time steps, we develop a novel algorithm able to couple two hybrid Chernoff tau-leap paths at different levels. Based on dual weighted residual expansion techniques, we also develop a new way of estimating the variance of the difference of two consecutive levels. This is crucial because the computational work required to stabilize the coefficient of variation of the sample variance estimator of the difference of two consecutive levels is often unaffordable. Our algorithm enforces the total error to be below a prescribed tolerance, TOL, with high probability, this is achieved with nearly optimal computational work. The computational complexity of our method is of the order of TOL^2. The numerical examples show substantial gains with respect to the previous single level approach and the SSA algorithm.

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I-7

Hybrid Adaptive Multilevel Monte Carlo Algorithm for Non Smooth Observables of Ito Stochastic Differential Equations.

Nadhir Ben Rached, Håkon Hoel and Raúl Tempone

The Monte Carlo forward Euler method with uniform time stepping is the standard technique to compute an approximation of the expected payoff of a solution of an Itô SDE. For a given accuracy requirement TOL, the complexity of this technique for well behaved problems, that is the amount of computational work to solve the problem, is $\mathcal{O}(\mathrm{TOL}^{-3})$. A new hybrid adaptive Monte Carlo forward Euler algorithm for SDEs with non-smooth coefficients and low regular observables is developed in this thesis. This adaptive method is based on the derivation of a new error expansion with computable leading-order terms. The basic idea of the new expansion is the use of a mixture of prior information to determine the weight functions and posterior information to compute the local error. In a number of numerical examples the superior efficiency of the hybrid adaptive algorithm over the standard uniform time stepping technique is verified. When a non-smooth binary payoff with either GBM or drift singularity type of SDEs is considered, the new adaptive method achieves the same complexity as the uniform discretization with smooth problems. Moreover, the new developed algorithm is extended to the MLMC forward Euler setting which reduces the complexity from $\mathcal{O}(\mathrm{TOL}^{-3})$ to $\mathcal{O}(\mathrm{TOL}^{-2}(\log(\mathrm{TOL}))^2)$. For the binary option case with the same type of Itô SDEs, the hybrid adaptive MLMC forward Euler recovers the standard multilevel computational cost $\mathcal{O}(\mathrm{TOL}^{-2}(\log(\mathrm{TOL}))^2)$. When considering a higher order Milstein scheme, a similar complexity result was obtained by Giles using the uniform time stepping for one dimensional SDEs. The difficulty to extend Giles' Milstein MLMC method to the multidimensional case is an argument for the flexibility of our new constructed adaptive MLMC forward Euler method which can be easily adapted to this setting. Similarly, the expected complexity $\mathcal{O}(\mathrm{TOL}^{-2}(\log(\mathrm{TOL}))^2)$ is reached for the multidimensional case and verified numerically.

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I-8

Multivariate polynomial approximation by discrete least squares with random evaluations

Giovanni Migliorati, Fabio Nobile and Raúl Tempone

We present the recent results achieved in $[1,2,3,4,5]$ concerning the analysis of the discrete least-squares method with random pointwise noise-free evaluations to approximate functions depending on multivariate random variables in the L2-probability sense. Suitable conditions between the number of evaluations and the dimension of the polynomial space are presented, to ensure stability and optimality of the polynomial approximation, depending on the underlying density of the random variables. Applications of the theoretical findings will be shown though some examples of partial differential equations with stochastic data.

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I-9

A Continuation MLMC algorithm

Nathan Collier, Abdul–Lateef Haji–Ali, Fabio Nobile, Erik von Schwerin and Raúl Tempone

We propose a novel Continuation Multi Level Monte Carlo (CMLMC) algorithm for weak approximation of stochastic models that are described in terms of differential equations either driven by random measures or with random coefficients. The CMLMC algorithm solves the given approximation problem for a sequence of decreasing tolerances, ending with the desired one. CMLMC assumes discretization hierarchies that are defined a priori for each level and are geometrically refined across levels. The actual choice of computational work across levels is based on parametric models for the average cost per sample and the corresponding weak and strong errors. These parameters are calibrated using Bayesian estimation, taking particular notice of the deepest levels of the discretization hierarchy, where only few realizations are available to produce the estimates. The resulting CMLMC estimator exhibits a non-trivial splitting between bias and statistical contributions. We also show the asymptotic normality of the statistical error in the MLMC estimator and justify in this way our error estimate that allows prescribing both required accuracy and confidence in the final result. Numerical examples substantiate the above results and illustrate the corresponding computational savings.

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Poster session II

Low-rank and sparse approximation/representation

II-1

Reduced Rank Adaptive Filtering in Impulsive Noise Environments

Hamza Soury, Karim Abed-Meraim and Mohamed-Slim Alouini

An impulsive noise environment is used in this paper. A new aspect of signal truncation is deployed to reduce the harmful effect of the impulsive noise to the signal. A full rank direct solution is derived followed by an iterative solution. The reduced rank adaptive filter is presented in this environment by using two methods for rank reduction. The minimized objective function is defined using the Lp norm. The results are presented and the efficiency of each algorithm is discussed.

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II-2

Dynamical low rank approximation of time dependent PDEs with random data

Eleonora Musharbash, Fabio Nobile and Tao Zhou

Stochastic partial differential equations suitably describe phenomena affected by uncertainty, due e.g. to measurement errors, limited data availability or intrinsic variability of the phenomenon itself. The approximation of differential problems with random parameters (e.g. coefficients, forcing terms, initial and boundary conditions) remains a challenging task when the dimension of the probability space is large and the solution features a complex dependence on the input parameters. In this context, we propose a Dynamically Orthogonal Field (DOF) approach, according to which the solution is approximated as a linear combination of a small number of deterministic orthogonal basis functions multiplied by random coefficients, both of them evolving in time in order to keep the dimensionality of the approximate problem low. The approximation solution is therefore forced to belong to a low dimensional manifold. If Ms denotes the manifold of all the functions of rank S, the approximate solution u(t) is obtained by projecting at each time step the residual of the governing equation onto the tangent space to Ms at u(t). Convergence properties of the DOF approach for parabolic equations with random coefficients are analyzed. The error analysis compares the DOF approximate solution with the best rank-S approximation (which corresponds to the truncated Karhunen-Lo‘eve expansion at each time t) and, under suitable conditions, it is shown that the error of the DOF approach can be bounded in terms of the best approximation error. The DOF approach and its convergence properties are assessed with several numerical examples.

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II-3

Kriging accelerated by orders of magnitude: combining low-rank covariance approximation with FFT-techniques

Alexander Litvinenko and Wolfgang Nowak

Computational power poses heavy limitations to the achievable problem size for Kriging. In separate research lines, Kriging algorithms based on FFT and low-rank representations of covariance functions have been developed, both leading to drastic speedup factors. The current study combines these ideas, reducing the computational complexity of Kriging to $\mathscr{O}(k_q m d L^* \log L^*)$, where k_q is the considered rank of approximation, m the number of measurement values, d the physical dimensionality, and L^* the number of lattice points along the longest edge of the regular d-dimensional lattice. For separable (factorized) covariance functions, rank $k_q = 1$ already yields exact results. These benefits can be fully exploited when leaving the final result in low-rank format, or when further low-rank operations follow. This occurs when evaluating the spatially averaged estimation variance or quadratic forms of the conditional covariance matrix, as they appear within optimal spatial design problems. Only outputting the final estimate as explicit map causes computational costs of $\mathscr{O}(k_q m n)$, where n is the number of estimation points. The current study assumes second-order stationarity and simple Kriging on a regular, equispaced lattice. Extensions to many other cases are straightforward.

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II-4

Computation of Periodic Orbits in Uncertain Navier-Stokes Flows

Olivier Le Maitre and Michael Schick

The determination of stable limit-cycles plays an important role for quantifying the characteristics of dynamical systems. In practice exact knowledge of model parameters is rarely available leading to parameter uncertainties, which can be modeled as random variables. This has the effect that the limit-cycles become stochastic themselves resulting in almost surely time-periodic solutions with a stochastic period. We introduce a numerical method for the computation of stable stochastic limit-cycles based on the Spectral-Stochastic-Finite-Element-Method using Polynomial Chaos (PC). The method overcomes the difficulties of Polynomial Chaos associated to the well known convergence breakdown for long time integration. To determine the limit cycles, a stochastic time scaling is first introduce to control the phase-drift of the stochastic trajectories, keeping the necessary PC expansion order low. Based on the re-scaled governing equations, stochastic initial condition and period are then determined such that the trajectories close after completion of one stochastic cycle. The numerical method is applied to the computation of vortex shedding for the flow around a circular cylinder with stochastic inflow boundary conditions. Results are verified by comparison to purely deterministic reference problems and demonstrate high accuracy up to machine precision in capturing the stochastic limit-cycle.

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II-5

Solution of Stochastic Nonlinear PDEs Using Automated Wiener-Hermite Expansion

Amnah Al-Juhani, Mohamed A. El-Beltagy

In this work, the Wiener-Hermite Expansion (WHE) is used in solving stochastic nonlinear PDEs with white-noise in the forcing term. The generation of the equivalent set of deterministic integro-differential equations is automated and hence allows for high order terms of WHE. The automation difficulties are discussed, solved and implemented to output the final system to be solved. A numerical Picard algorithm is suggested to solve the resulting system. The automated WHE is applied on the 1D diffusion equation and on the heat equation. The results are compared with previous research solutions obtained with WHEP (WHE with perturbation) technique. In this case, the WHE solutions are considered as a limit of the WHEP solutions with infinite number of corrections. The automation is extended easily to account for white-noise of higher dimension and for general nonlinear PDEs.

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II-6

Analysis and computation of acoustic and elastic wave equations in random media

Motamed Mohammed, Fabio Nobile, Raúl Tempone

We propose a stochastic collocation method for solving the second order acoustic and elastic wave equations in heterogeneous random media subjected to deterministic boundary and initial conditions. We assume that the medium consists of non-overlapping sub-domains with smooth interfaces. In each sub-domain, the materials coefficients are smooth and given or approximated by a finite number of random variable. One important example is wave propagation in multi-layered media with smooth interfaces. The numerical scheme consists of a finite difference or finite element method in the physical space and a collocation in the zeros of suitable tensor product orthogonal polynomials (Gauss points) in the probability space. We provide a rigorous convergence analysis and demonstrate different types of convergence of the probability error with respect to the number of collocation points under some regularity assumptions on the data. In particular, we show that, unlike in elliptic and parabolic problems, the solution to hyperbolic problems is not in general analytic with respect to the random variables. Therefore, the rate of convergence is only algebraic. A fast spectral rate of convergence is still possible for some quantities of interest and for the wave solutions with particular types of data. We also show that the semi-discrete solution is analytic with respect to the random variables with the radius of analyticity proportional to the grid/mesh size h. We therefore obtain an exponential rate of convergence which deteriorates as the quantity hp gets smaller, with p representing the polynomial degree in the stochastic space. We have shown that analytical results and numerical examples are consistent and that the stochastic collocation method may be a valid alternative to the more traditional Monte Carlo method.

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II-7

Quasi-optimal sparse-grid approximations for elliptic PDEs with stochastic coefficients

Fabio Nobile, Lorenzo Tamellini and Raúl Tempone

Partial differential equations with stochastic coefficients conveniently model problems in which the data of a given PDE are affected by uncertainty, due e.g. to measurement errors, limited data availability or intrinsic variability of the described system. Here we consider the case of an elliptic PDE with diffusion coefficient depending on N random variables $y_1,\dots,y_N$. In this context, the solution u of the PDE at hand can be seen as a random function, $u = u(y_1,\dots,y_N)$, and common goals include computing its mean and variance, or the probability that it exceeds a given threshold. This could be achieved with a straightforward Monte Carlo method, that may however be very demanding in terms of computational costs. Methods based on polynomial approximations of $u(y_1,\dots,y_N)$ have thus been introduced, aiming at exploiting the possible degree of regularity of u with respect to $y_1,\dots,y_N$ to alleviate the computational burden. Such polynomial approximations can be obtained e.g. with Galerkin projections or collocation methods over the parameters space. Although effective for problems with a moderately low number of random parameters, these methods suffer from a degradation of their performance as the number of random parameters increase ("curse of dimensionality"). Minimizing the impact of the "curse of dimensionality" is therefore a key point for the application of polynomial methods to high-dimensional problems. In this poster we illustrate a possible strategy to carry out such task when building sparse grids approximation of u. In particular, we will consider a "knapsack approach", in which we estimate the cost and the "error reduction" contribution of each possible component of the sparse grid, and then we choose the components with the highest "error reduction"/cost ratio. The estimates of the "error reduction" are obtained by a mixed "a-priori"/"a-posteriori" approach, in which we first derive a theoretical bound and then tune it with some inexpensive auxiliary computations. We will present some theoretical convergence results as well as numerical results showing the efficiency of the proposed approach.

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II-8

Higher-order Solution of Stochastic Diffusion equation with Nonlinear Losses Using WHEP technique

Mohamed A. El-Beltagy and Noha A. Al-Mulla

In the current work, the Wiener-Hermite Expansion with perturbation (WHEP) technique of order and number of corrections will be used to solve the stochastic diffusion equation with nonlinear losses. The solutions will be obtained analytically, using Mathematica, and numerically using the finite-volume method (FVM). The mean and variance of higher-order non-Gaussian solutions are obtained and compared with lower order ones. The proposed techniques are shown to be efficient in estimating the solutions of stochastic nonlinear PDEs.

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Poster session III

Bayesian Inference methods

III-1

Fast Estimation of Expected Information Gain for Bayesian Experimental Design Based on Laplace Approximation

Quan Long, Marco Scavino, Raúl Tempone and Suojin Wang

In this work, we extend the Laplace method in experimental designs to the general case where the model parameters cannot be determined completely by the data from the proposed experiments. We carry out the Laplace approximations in the directions orthogonal to the null space of the Jacobian matrix of the model with respect to the parameters, so that the information gain can be reduced to an integration against the marginal density of the transformed parameters which are not determined by the experiments. Furthermore, the expected information gain can be approximated by an integration over the prior, where the integrand is a function of the posterior covariance matrix projected over the forementioned orthogonal directions. To deal with the issue of dimensionality in a complex problem, we use either Monte Carlo sampling or sparse quadratures for the integration over the prior probability density function, depending on the regularity of the integrand function. We demonstrate the accuracy, efficiency and robustness of the proposed method via several nonlinear under determined test cases.

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III-2

A Bayesian setting for an inverse problem in heat transfer

Zaid Sawlan, Marco Scavino and Raúl Tempone

This work develops a Bayesian setting to infer thermal conductivity, the material parameter that characterizes the heat equation in a boundary-initial condition problem. We first derive a conditional likelihood function for the forward problem, given the values of the temperature at the boundaries and using the inner measurements as data. Then, we marginalize this likelihood with respect to adequate Gaussian priors on the time dependent Dirichlet boundary. We then propose two Bayesian models for inference, assuming that either the thermal conductivity parameter is a lognormal random variable or it is a space dependent only, stationary lognormal random field respectively. Finally, we use synthetic data to carry out the inference and even to estimate the expected information gain for a designed experiment. A Laplace type of approximation is used to accelerate the numerical computations, avoiding a costly MCMC alternative.

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III-3

Non-Linear Bayesian update of surrogate model

Alexander Litvinenko and Hermann G. Matthies

The Bayesian Update is quite vital for uncertainty quantification. With BU we can take into account the given measurements of our physical model and update a priori probability density function (which is very often far away from the truth) of the uncertain parameter. The standard full BU is based on sampling and sampling is not always acceptable or possible. In addition, it can require a very large number of samples and is expensive. This motivated us to develop sampling-free non-linear Bayesian update (NLBU). We derive it from the variational problem associated with conditional expectation. Whereas the linear BU is a linear function of the prediction mismatch, here we used higher order polynomials. An important intermediate subproblem which appears during the linear BU is increasing of the stochastic dimension after each update (curse of dimensionality). The reason is the new random variables which come from the random measurement noise. As an example we took the chaotic Lorenz 84 model.

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III-4

Multiscale Bayesian model for uncertainty quantification in porous media

Matteo Icardi, Ivo Babuska, Serge Prudhomme and Raúl Tempone

Fluid flows and transport processes in porous media are commonly described by simplified averaged macro-scale equations and effective parameters. However, there has been a growing interest in more detailed descriptions of the flow at the pore-scale in the recent years. This is due mainly to the complex multiscale and multiphysics nature of the applications and to the lack of knowledge on macro-scale parameters and models that cause high uncertainty on the final quantities of interest. This is the case, for example, of the dispersion and reaction of particles and contaminants in groundwater, where the estimation of parameters and transport properties can vary by orders of magnitude. Another important example is the multi-phase flow problem in carbon storage and sequestration applications. To address these problems, two main directions can be undertaken: on one hand there is a growing effort to develop uncertainty quantification tools based on stochastic partial differential equations that explicitly express the lack of knowledge and variability in model parameter in terms of random variables and random fields. On the other hand, all the sources of uncertainty must be better investigated, by means of detailed fine-scale experimental and computational studies, to understand their physical basis and stochastic parametric representation. In this work we study the uncertainty of macro-scale flow and transport parameters coming from the inner pore-scale structure of granular packings, implicitly parametrized by input parameters of deposition algorithms. A set of realizations of random porous media are generated and studied in terms of physical and transport properties (porosity, tortuosity, permeability, dispersivity) by solving the flow equations in the void space. These results can be used to understand more clearly the dependence of the parameters on the flow regime and porous medium properties and to give prior information to the stochastic description of the flow. The pore-scale results are systematically integrated in a Hierarchical Bayesian framework and combined with prior spatial information and data coming from laboratory and field scale results. Direct numerical upscaling and Bayesian inversion are used to calibrate simplified macro-scale parameters while the prediction at arbitrary spatial locations can be achieved using statistical interpolation techniques, e.g., Kriging, in the same Bayesian framework. The resulting macro-scale random field can be used to estimate the expected value and the uncertainty of macro-scale quantities of interest, and to design and optimize sampling, laboratory and pore-scale investigations for groundwater remediation, oil recovery and carbon storage problems.

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III-5

Ensemble Bayesian Filters for Efficient Multi-Data Reservoir History Matching

Klemens Katterbauer, Fabio Ravanelli, Mohamad ElGharamti, Boujemaa Fquih and Ibrahim Hoteit

With rising demand for oil and gas and increased complexity of exploration projects, reservoir management is playing a critical role for optimizing recovery rates, increasing return on investment and ensuring stable production rates. To achieve these goals, a more detailed understanding and accurate mapping of the reservoir formation is essential for forecasting fluid propagation, determining water saturation levels, estimating remaining oil in place, and implementing enhanced recovery techniques for managing production levels. Reservoir modeling is crucial for simulating and understanding the Earths subsurface formation and is based on gathered reservoir data for estimating reservoir properties such as permeability and porosity. While production data have been employed for decades for calibrating models and the estimation of reservoir parameters, the petroleum industry has been focusing on overcoming the shortcomings of the sparsely sampled production data via the incorporation of additional data sets. Time-lapse seismic data have enabled engineers to map more precisely hydrocarbon and fluid reservoirs and track their evolution. With the challenges faced by seismic methods in accurately distinguishing between hydrocarbons and injected fluids, electromagnetic (EM) methods have attracted significant attention to exploit the sharp contrast in conductivity between hydrocarbons and injected water. Recently, gravity as well as magnetic measurement techniques assumed a critical role providing vital information about the strong density variation between gas and fluids, while satellite techniques, such as InSAR, have been shown to provide information about changes in the reservoir formation pressure levels. The conventional approach to incorporate these data into the reservoir, although known as the history matching process, have been to invert them first, without knowledge of the flow, and then employing them as constraints in the reservoir simulation. Reservoir history matching became a quintessential tool for quantifying uncertainties in oil and gas production. Uncertainty quantification is indispensable to determine the financial feasibility and economics of exploration projects and provide accurate forecasts. Standard approaches to history matching have been to manually or semi-automatically adjust reservoir parameters to match the observed production data at the wells. With rising complexity and increase in the amount of data, data assimilation methods became very popular for efficient estimation of reservoir properties from observed reservoir data. We present a general framework for using advanced ensemble-based Bayesian filtering techniques in order to simultaneously incorporate all available reservoir observation, such as production, seismic, EM, gravimetry, magnetic and satellite data, into the history matching process. Our goal is to enhance the history matching process and to determine the best possible picture of the reservoir using the complementarity of the information provided by the different reservoir data sets. Ensemble filtering techniques have been proven efficient, versatile and accurate for estimating reservoir properties. Amongst the filters, the EnKF has been widely applied due to its simplicity with the EnKS becoming more attractive for real data applications due to its smoothing properties. The SEIK has been recently introduced for reservoir history matching due to its favorable properties of coping with large number of observations. We present results from extensive studies for different reservoir types demonstrating the efficiency of the proposed system in significantly enhancing production forecasts and reservoir parameters estimation, providing a vital tool for enhanced reservoir management and uncertainty quantification.

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III-6

Data-Driven Model Reduction for the Bayesian Solution of Inverse Problems

Tiangang Cui, Youssef Marzouk and Karen Willcox

A novel data-driven model reduction technique is developed for solving large-scale inverse problems. The proposed technique exploits the fact that the solution of the inverse problem often concentrates on a low dimensional manifold. Unlike typical MCMC approaches for solving the inverse problem, our approach avoids repeated evaluation of expensive forward models by coupling the inference algorithm with the reduced-order model. This maintains the accuracy of the inference and also results in a lower-dimensional reduced model than obtained with the typical POD approach.

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Poster session IV

Green Wireless Communication

IV-1

A Coalition Formation Game for Transmitter Cooperation in Uplink Communications

Ali Chelli, Hamidou Tembine and Mohamed-Slim Alouini

The SC-FDMA (single-carrier frequency division multiple access) is the access scheme that has been adopted by 3GPP (3rd generation partnership project) for the LTE (long term evolution) uplink. The SC-FDMA is an attractive alternative to OFDMA (orthogonal frequency-division multiple access) especially on the uplink owing to its low peak-to-average power ratio. This fact increases the power efficiency and reduces the cost of the power amplifiers at the mobile terminals. The use of SC-FDMA on the uplink implies that the base station allocates a single subcarrier to each user. This results in the limitation of the achievable rate on the uplink. In this work, we propose a coalition game between mobile terminals that allows them to improve their performance by sharing their subcarriers without creating any interference for each other. The proposed scheme allows a fair use of the subcarriers and leads to a significant capacity gain for each user. The cooperation between the nodes is modelled using coalitional game theory. In this game, each coalition tries to maximize its utility in terms of rate. In the absence of cooperation cost, it can be shown that the grand coalition is sum-rate optimal and stable, i.e., the mobile terminals have no incentive to leave the grand coalition.

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IV-2

Modeling of MAI in UWB System Using Multivariate Generalized Gaussian Distribution

Qasim Z. Ahmed, Ki-Hong Park and Mohamed-Slim Alouini

Multivariate generalized Gaussian density (MGGD) is used to approximate the multiple access interference (MAI) and additive white Gaussian noise in pulse-based ultrawide bandwidth (UWB) system. The MGGD probability density function (pdf) is shown to be a better approximation of a UWB system as compared to Gaussian, Laplacian and Gaussian-Laplacian mixture (GLM). The similarity between the simulated and the approximated pdf is measured with the help of modified Kullback-Leibler distance (KLD). It is also shown that MGGD has the smallest KLD as compared to Gaussian, Laplacian and GLM densities. Finally, a receiver based on the principles of minimum bit error rate is designed for the MGGD pdf.

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IV-3

Efficient Particle Swarm Optimization Algorithm for Optimized LTE Base Station Deployment

Hakim Ghazzai, Elias Yaacoub and Mohamed-Slim Alouini

Base station deployment in cellular networks is one of the most fundamental problems in network design. This paper proposes an efficient method for cell planning problem for the fourth generation 4G-LTE cellular networks. In this approach, we aim to satisfy both coverage and cell capacity constraints simultaneously by formulating a practical optimization problem. We start by performing a traditional coverage and capacity dimensioning to identify the initial required number of base stations. Afterwards, we implement a particle swarm optimization algorithm in order to optimize the base station locations such that we satisfy both problem constraints in the area of interest which can be divided into several subareas with different user densities. Then, an iterative approach is executed to eliminate eventual redundant base stations. We have also performed Monte Carlo simulations to study the performance of the proposed scheme for multiple scenarios and computed the average number of users in outage. Results show that our proposed approach respects in all cases the desired network quality of services even for large-scale dimension problems.

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IV-4

Threshold based Adaptive Detection for Cooperative Wireless Sensor Networks

Abdulrahman Abuzaid, Qasim Z. Ahmed and Mohamed-Slim Alouini

Efficient receiver designs for wireless sensor networks (WSNs) are becoming increasingly important. In previous work, cooperative WSNs communicated with the use of L sensors. As the constraint receiver can only process U out of L sensors, channel shortening and reduced-rank techniques were employed to design the preprocessing matrix. In this paper, a receiver structure is proposed which combines the joint iterative optimization (JIO) algorithm and our proposed threshold selection criteria. This receiver structure assists in determining the optimal U_{opt}. Furthermore, this receiver provides the freedom to choose $U \leq U_{opt}$ for each frame depending upon the tolerable difference allowed for mean square error (MSE). Our study and simulation results show that by choosing an appropriate threshold, it is possible to gain in terms of complexity savings without affecting the BER performance of the system.

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IV-5

Low Complexity Transmission Scheme with Full Diversity for Two-Path Relay Networks

Muhammad Mehoob Fareed, Hong-Chuan Yang and Mohamed-Slim Alouini

In this poster, we present a new low complexity scheme for two-path relay network to harvest maximum achievable diversity. We analyze the performance of the resulting two-path relay network for arbitrary locations by calculating the symbol error rate and diversity order. It is shown that with this newly proposed scheme, two-path relay networks can mimic a 2x2 multiple-input mulitple-output system and achieve full diversity order of four. Simulations results are provided to verify and illustrate the analytical results.

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IV-6

On Achievable Rates of Cognitive Radio Networks Using Multi-Layer Coding

Lokman Sboui, Zouheir Rezki and Mohamed-Slim Alouini

We study the impact of adopting a multi-layer coding (MLC) strategy, i.e., the so-called broadcast approach (BA) on the throughput of Cognitive Radio (CR) spectrum sharing systems for general fading channels. First, we consider a scenario where the secondary transmitter, apart from the statistics, has no channel state information (CSI) of the cross link and its own link. We show that using BA improves the cognitive achievable rate compared to the outage rate provided by a single layer coding (SLC). In addition, we observe numerically that 2-Layer coding achieves most of the gain for Rayleigh fading. Then, we consider a situation where the secondary transmitter has a partial CSI about its own link through quantized CSI. Again, we compute the secondary achievable rate adopting the BA and highlight the improvement over SLC. Numerical results show that the advantage of MLC decreases as the rate of the feedback link increases.

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IV-7

Capacity of Some Fading Channels in the Low Power Regime with Imperfect Channel State Information

Fatma Benkhelifa, Zouheir Rezki, Mohamed-Slim Alouini

The low power regime has attracted various researchers in the information theory and communication communities to understand the performance limits of wireless systems. Indeed, the energy consumption is becoming one of the major limiting factors in wireless systems. As such, energy-efficient wireless systems are of major importance to the next generation wireless systems designers. The capacity is a metric that measures the performance limit of a wireless system. The study of the ergodic capacity of some fading channels in the low power regime is the main subject of this poster. We assume that the transmitter and the receiver have possibly imperfect knowledge of the channel state information (CSI). We provide an explicit characterization of how the capacity scales as function of the signal-to-noise ratio (SNR) in the low power regime. This allows us to characterize the gain due to the perfect knowledge compared to no knowledge of the channel state information at the transmitter. We study the ergodic capacity of a maximum ratio combining (MRC) Rician fading channel with perfect CSI at the transmitter and at the receiver. We show that one-bit CSI feedback at the transmitter is enough to achieve this capacity using an on-off power control scheme. We study the capacity of Multiple-Input Multiple-output (MIMO) Gaussian channels that undergo Rayleigh and Rician fading with imperfect CSI at the transmitter and/or the receiver. We show that the capacity loss due to the channel estimation at the transmitter at low SNR is function of the estimation error variance. Whereas, we show that the channel estimation at the receiver at low SNR is not crucial. Finally, we study the capacity of Nakagami-m fading channel with perfect CSI at both the transmitter and the receiver under delay quality of service (QoS) constraints, namely the effective capacity. We show that the effective capacity converges to ergodic capacity, independently of any QoS constraint, in the very low power regime.

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IV-8

Transmit Power Optimization for Green Multihop Relaying over Nakagami-m Fading Channels

Itsikiantsoa Randrianantenaina, Mustapha Benjillali , and Mohamed-Slim Alouini

We investigate the optimal transmit power strategy to maximize the energy efficiency of a multihop relaying network. Considering the communication between a source and a destination through multiple Amplify-and-Forward relays, we first give the expression of the total instantaneous system energy consumption. Then, we define the energy efficiency in our context and obtain its expression in closed-form when the communication is over Nakagami-m fading channels. The analysis yields to the derivation of a global transmit power strategy where each individual node is contributing to the end-to-end overall energy efficiency. Numerical results are presented to illustrate the analysis. Comparison with Monte Carlo simulation results confirms the accuracy of our derivations, and assesses the gains of the proposed power optimization strategy.

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Poster session V

Computational Electro-Magnetics

V-1

MOT Solution of Time Domain PMCHWT Integral Equation for Conductive Dielectric Scatterers

Ismail E. Uysal, Huseyin A. Ulku and Hakan Bagci

A time domain surface integral equation (TD-SIE) solver is proposed for analyzing transient electromagnetic interactions on conductive dielectric scatterers. The proposed solver utilizes the well-known Poggio-Miller-Chan-Harrington-Wu-Tsai (PMCHWT) SIE formalism to describe the scattered fields in terms of equivalent surface electric and magnetic currents introduced at material interfaces and the time domain Green function of the unbounded conductive medium. Equivalent currents are expanded in terms of Rao-Wilton-Glisson (RWG) functions in space and polynomial interpolants in time. Inserting these expansions into the TD-SIE and Galerkin testing the resulting equation at time samples results in a matrix system of equations. This matrix system is solved for current expansion coefficients using the marching-on-in-time (MOT) technique. The PMCHWT formulation allows for modeling of multilayered conductive scatterers, which is not possible with the existing MOT-TD-SIE solver developed for single conductive objects.

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V-2

On the DC Loop Modes in MOT Solution of Time Domain Electric Field Integral Equation

Yifei Shi, Mingyu Lu and Hakan Bagci

When marching-on-in-time (MOT) method is applied to solve the time domain electric field integral equation, spurious internal resonant and DC loop modes are always observed in the solution. The internal resonant modes have recently been studied in; this letter investigates the DC loop modes. Like internal resonant modes, DC loop modes, in theory, should not be observed in the MOT solution since they do not satisfy the relaxed initial conditions; and their appearance is attributed to numerical errors. It is discussed in this letter that, the dependence of spurious DC loop modes on numerical errors is substantially different from that of spurious internal resonant modes. More specifically, when Rao-Wilton-Glisson functions and Lagrange interpolation functions are used as spatial and temporal basis functions respectively, errors due to space-time discretization have zero impact on spurious DC loop modes. Numerical experiments indeed support this discussion and demonstrate that the numerical errors due to the approximate solution of the MOT matrix system have dominant impact on spurious DC loop modes in the MOT solution.

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V-3

A Hybrid Time-Domain Discontinuous Galerkin-Boundary Integral Method for Electromagnetic Scattering Analysis

Ping Li, Yifei Shi, Li Jun Jiang and Hakan Bagci

A scheme hybridizing discontinuous Galerkin time-domain (DGTD) and time-domain boundary integral (TDBI) methods for accurately analyzing transient electromagnetic scattering is proposed. Radiation condition is enforced using the numerical flux on the truncation boundary. The fields required by the flux are computed using the TDBI from equivalent currents introduced on a Huygen's surface enclosing the scatterer. The hybrid DGTDBI ensures that the radiation condition is mathematically exact and the resulting computation domain is as small as possible since the truncation boundary conforms to scatterer's shape and is located very close to its surface. Locally truncated domains can also be defined around each disconnected scatterer additionally reducing the size of the overall computation domain. Numerical examples demonstrating the accuracy and versatility of the proposed method are presented.

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V-4

An Accurate and Stable MOT Solver for Time Domain EFIE, MFIE, and CFIE using on Exact Integration Technique

Yifei Shi, Mingyu Lu and Hakan Bagci

An exact integration of double surface integrals in marching-on-in-time solver for time domain electric/magnetic field integral equation is presented. The double spatial surface integrals over the observation and the source patches are transformed to a set of spatial surface integrals over a determined geometric domain. For general case, all the integrals including piecewise polynomial temporal functions can be converted to several arc and line contour integrals according to the spatial shape between the geometric domain and temporal circular cuts. All these arc and line integrals have analytical solutions by recursive formulations and are be derived analytically. Only one-dimensional Gaussian quadrature is needed. For the near singularity from magnetic field integral equation, an analytical expression is adopted to extract the logarithmic singularity appears in the one-dimensional Gaussian quadrature. Additionally in self-term case of electric field integral equation, the closed form of all integrals can be achieved in a fully analytical form without numerical approximation. The numerical results show that all the results are accurate and stable.

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V-5

Solution of 2D Electromagnetic Inverse Scattering Problem Using Iterative Shrinkage-Thresholding Algorithms

Abdulla Desmal and Hakan Bagci

It is well known that second-norm regularizers, which are used to alleviate the ill-possedness of the electromagnetic inverse scattering problem, promote the smoothness in the solution. These regularizers, therefore, cannot efficiently produce accurate results when applied in domains with sharp variations, discontinuities, or sparse content. In these cases, priori knowledge of the domains sparseness could be used to alleviate the ill-possedness via the use of a zeroth or first-norm regularizer. In this work, several gradient-based iterative shrinkage thresholding algorithms that have been developed for minimizing cost functions with zeroth and first-norm regularizers are used in conjunction with the Born iterative method to solve the two-dimensional inverse electromagnetic scattering problem. Numerical results demonstrate the superiority of the proposed framework over the Born iterative method that uses second-norm regularizers when they are applied in sparse/sparsified domains; the dielectric permittivity/conductivity profiles recovered using the proposed framework are sharper and more accurate.

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V-6

Preconditioned Inexact Newton for Nonlinear Sparse Electromagnetic Imaging

Abdulla Desmal and Hakan Bagci

Newton class of algorithms have been intensively studied in nonlinear microwave imaging due to their quadratic convergence rate and their ability to recover microwave images with high contrast. In most of the previous studies, Newton methods where implemented in conjunction with smooth recovering optimization tools. However, smooth regularization performs poorly with sparse content or sharp variation domains. In this work, an Inexact Newton algorithm is implemented in conjunction with linear sparse optimization algorithm. A preconditioning procedure is proposed to aid the convergence of the sparse iterative solver. Additionally, the scheme of the Inexact Newton is modified to remove the small ripples generated by the Newton modification.

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V-7

Stabilizing MOT Solution of TD-VIE for High-contrast Scatterers using Accurate Extrapolation

Sadeed B. Sayed, Huseyin A. Ulku and Hakan Bagci

The marching on-in-time (MOT) based time domain volume integral equation (TD-VIE) solvers suffer from instabilities, especially when they are applied in analyzing electromagnetic wave interactions on high contrast dielectric scatterers. It is well-known that using band-limited interpolation functions (BLIFs) in the expansion of unknown fields helps to stabilize the MOT solution. Unfortunately, BLIFs are two sided, i.e., they require ”future” field samples for interpolation, resulting in a non-causal MOT system. The non-causality can be resolved using an extrapolation scheme that estimates the future values of the fields from their past values. In this work, an accurate, stable and band-limited extrapolation scheme is proposed. This extrapolation scheme uses complex exponents, rather than commonly used harmonics, so that propagating and decaying mode fields inside the dielectric scatterers are accurately modeled. Numerical results indeed demonstrate that the resulting MOT-TD-VIE solver maintains its stability and accuracy even when applied to the analysis of wave interactions on high contrast scatterers.

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V-8

An Explicit and Stable MOT Solver for Time Domain Volume Electric Field Integral Equation

Sadeed B. Sayed, Huseyin A. Ulku and Hakan Bagci

An explicit yet stable marching-on-in-time (MOT) solver that employs a predictor-corrector scheme to efficiently solve the time domain volume electric field integral equation (TD-VEFIE) is proposed. Spatial discretization of the TD-VEFIE is carried out in the same way as its ”classical” implicit counterparts but the time marching is constructed in the form of a traditional PE(CE)m scheme. The stability and accuracy of the time marching are then controlled using successive over relaxation (SOR) applied at each repetition of the corrector step. As opposed to its implicit counterpart, the explicit solver requires at every time step inversion of a matrix system with a Gram matrix that is sparse and well-conditioned regardless of time step size. Additionally, unlike the classical explicit MOT solvers, the proposed solver can work with large time steps as in its implicit counterpart. Numerical results indeed demonstrate that it provides the MOT solution faster especially for low-contrast scatterers compared to classical implicit solvers.

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Poster session VI

Reactive Computational Fluid Dynamics

VI-1

Spectral uncertainty analysis of combustion reaction systems using sparse adaptive polynomial chaos expansions

Daesang Kim, Jie Han, Fabrizio Bisetti and Omar Knio

We applied a sparse adaptive pseudo-spectral method to two model reaction systems, H2 oxidation and methane ignition in shock tubes, for the investigation of uncertainty characteristics in the reaction mechanisms of the model systems. The non-intrusive algorithm creates polynomial chaos expansions of the reaction systems with orthogonal polynomial terms, and the expansion coefficients are determined through a weighted inner product which requires the reaction model realizations at many quadrature points. The method achieved its fast and efficient performance by adopting sparse adaptive quadrature grids based on the notions of arbitrary admissible Smolyak multi-index sets. The application of the method provided sensitivities and uncertainty propagations between measurements and reaction rate parameters of the model systems as well as screening of active reaction rate parameters. Also provided were efficient surrogate polynomial models, which enabled to avoid intensive computations of simulation models to perform least squares and Markov Chain Monte Carlo to study the uncertainties in the model systems.

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VI-2

Optimal Design and Model Validation for Combustion Experiments in a Shock Tube

Quan Long, Daesang Kim, Raúl Tempone, Fabrizio Bisetti, Aamir Farooq, Omar Knio and Serge Prudhomme

We develop a Bayesian framework for the optimal experimental design of the shock tube experiments which are being carried out at the KAUST Clean Combustion Center. The unknown parameters are the pre-exponential parameters and the free energies in the reaction rate functions. The control parameters are the initial hydrogen concentration and the temperature. There are several tasks in this research. First, we build a polynomial based surrogate model for the reactions in the shock tube. Second, we use a novel MAP based approach to estimate the expected information gain in the proposed experiments and select the best experimental set-ups corresponding to the optimal expected information gains. Third, we use the synthetic data to carry out virtual validation of our methodology. The work to be done soon includes validation using real data from the laboratory experiments and extending experimental design methodology to the cases where the control parameters are noisy.

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VI-3

Simulation of soot size distribution in an ethylene counterflow flame

Kun Zhou, Ahmed Abdelgadir and Fabrizio Bisetti

Soot formed during the rich combustion of fossil fuels is an undesirable pollutant and health hazard. A newly developed Monte Carlo method is used to simulate the soot formation in a counterflow diffusion flame of ethylene. The simulation uses a new reaction mechanism, recently developed at KAUST, which focuses on modeling the formation of large polycyclic aromatic hydrocarbons (PAHs) up to coronene ($C_{24}H_{12}$). Nascent soot particles are assumed to form from the collision of eight different PAH molecules. Soot surface growth includes the hydrogen-abstraction-C_2H_2-addition mechanism and the condensation of the PAHs. Soot coagulation is in the free-molecular regime because particles are small (no more than a hundred nanometer). The coupling between vapor consumption and soot formation is handled by an interpolative moment method. Soot particle diffusion is found negligible throughout the counterflow flame, except for a very narrow region right around the stagnation plane. The soot particle size distribution (PSD) generally exhibits a bimodal shape. The first peak corresponds to a large number of nascent particles, while the second peak results from the competition between nucleation and coagulation. Surface growth affects the PSD quantitatively, but does not change the modality. A comparison with experimental data is also provided.

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Poster session VII

Other Applications

VII-1

Large scale modeling, simulation and improved models for CO2 storage

Bilal Saad, Raúl Tempone and Serge Prudhomme

CO2 sequestration is a complex multiphysics process, in which multiphase multicomponent flows play critical role. The fact that the CO2 should be stored for many thousands of years implies that full scale experiments are not possible, and computer simulation is the main approach for exploring the feasibility of different CO2 storage options. Various risks exist in CO2 sequestration, the most important being (i) CO2 leakage through cap-rock failure, faults, abandoned wells, (ii) Brine displacement and infiltration into drinking water aquifers. To address these problems, an important effort, in this work, addressed for the modeling and simulation of the injection and storage process, in order to evaluate the sequestration potential and the long term behavior of the selected geologic formations. On the other hand, quantification of the risks and uncertainties is of ultimate importance for the decision makers when evaluating the storage approaches. In this part, statistical uncertainty addressed to better understand the influence of the model parameters (permeability, porosity, diffusion) on specific features and to subject the models to a thorough Verification and Validation process in order to assess their predictive capabilities.

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VII-2

The Red Sea Forecasting System

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Despite its importance to the world community for a variety of socio-economical reasons and the presence of extensive coral reef gardens along its shores, the Red Sea remains one of the most under-studied large marine physical and biological systems in the global ocean. We present our efforts to build advanced modeling, data assimilation, and uncertainty quantification capabilities for the Red Sea, which is part of the newly established Saudi ARAMCO Marine Environmental Research Center aiming at studying and forecasting the circulation and the environment of the Red Sea. The Red Sea modeling system compromises a regional and nested very high resolution costal MIT general circulation models (MITgcm) to simulate the general circulation at various spatial scales, a 10km resolution Weather Research Forecasting (WRF) model to simulate the atmospheric conditions, a 4km resolution European Regional Seas Ecosystem Model (ERSEM) to simulate the ecosystem, and a 1km resolution WAVEWATCH-III model to simulate the wind driven surface waves conditions. We have also implemented an oil spill model, and a probabilistic dispersion and larval Connectivity Modeling System (CMS) based on a stochastic Lagrangian framework. The Red Sea MITgcm, WRF and ERSEM models have also been equipped with advanced fully parallel Ensemble-based Kalman Filtering (EnKF) tools capable of assimilating all multivariate satellite and in-situ data sets that have been collected or will be collected in the future. EnKFs have been proven successful for ocean data assimilation, efficiently propagating and reducing uncertainties of large scales ocean simulations. The important role of uncertainties is now increasingly recognized in the ocean forecasting community for proper decision-making and risk management. In an EnKF, the forecasts and their uncertainties come as ensembles of mode simulations. Incoming ocean observations are then used to quantify and reduce the uncertainties in the forecasts. We have also built an advanced visualization framework to enable users to easily extract and identify the important information from such large ensembles. We will give an overview of our Red Sea modeling and forecasting system, discuss the choice of methods, summarize our major findings so far and our present future plans.

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VII-3

Multiscale Modeling of Wear Degradation in Cylinder Liners

Alvaro Moraes, Raúl Tempone and Pedro Vilanova

Every mechanical system is naturally subjected to some kind of wear process that, at some point, will cause failure in the system if no monitoring or treatment process is applied. Since failures often lead to high economical costs, it is essential both to predict and to avoid them. To achieve this, a monitoring system of the wear level should be implemented to decrease the risk of failure. In this work, we develop a multiscale indirect inference methodology for state-dependent Markovian pure jump processes that allows us to model the evolution of the wear level, and to identify when the system reaches some critical level that triggers a maintenance response. Since the likelihood function of a discretely observed pure jump process does not have an expression that is simple enough for standard non-sampling optimization methods, we approximate this likelihood by expressions from upscaled models of the data. We use the Master Equation to assess the goodness-of-fit and to compute the distribution of the hitting time to the critical level.

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VII-4

A stochastic multiscale method for the elastodynamic wave equation arising from fiber composites

Ivo Babuska, Mohammed Motamed, Raúl Tempone

We present a stochastic multilevel global-local algorithm for computing elastic waves propagating in fiber-reinforced composite materials. Here, the materials properties and the size and location of fibers may be random. The method aims at approximating statistical moments of some given quantities of interest, such as stresses, in regions of relatively small size, e.g. hot spots or zones that are deemed vulnerable to failure. For a fiber-reinforced cross-plied laminate, we introduce three problems (macro, meso, micro) corresponding to the three natural scales, namely the sizes of laminate, ply, and fiber. The algorithm uses the homogenized global solution to construct a good local approximation that captures the microscale features of the real solution. We perform numerical experiments to show the applicability and efficiency of the method.

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VII-5

Emulation of Global 3D Spatio-Temporal Temperature: A Distributed Computing Approach to Model 1 Billion Data Points

Stefano Castruccio and Marc G. Genton

The use of Statistics for reproduction (emulation) of climate model output is a field that has seen increasing interest from both the geophysical and policy making community. The use of empirical statistical models for data generation instead of time-consuming Partial Differential Equations is a promising avenue for providing simple, fast, and easy-to-use tools for decision making. The main challenge of fitting a statistical model to computer generated output in space and time is the size: covariance matrices describing the interaction between all data points easily become not storable in RAM memories, thus making data reduction or model simplification a necessity. In this poster we show how the use of a large number of processors allows for emulation of three dimensional temperature fields on the Earth without data reduction. By distributing the covariance storage across multiple cores in a cluster, it becomes possible to fit models with data of unprecedented size. Here we show how it is possible to fit a non-trivial model for a data set of 1 billion data points with a covariance matrix having 10^{18} entries.

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VII-6

Mean Field Game for Marriage

Dario Bauso, Ben Mansour Dia, Boualem Djehiche, Hamidou Tembine and Raúl Tempone

The myth of marriage has been and is still a fascinating historical societal phenomenon. Paradoxically, the empirical divorce rates are at an all-time high. In order to design and evaluate interventions, theoretical understanding of marital stability and dissolution is crucial. This article describes a unique paradigm for preserving relationships and marital stability from mean-field game theory. The approach is quite general for modeling social interaction, and can be applied to empirical data generated over time. We show that optimizing the long-term well being via effort and society feeling state distribution will help in stabilizing relationships. The optimal effort of the mean-field sentimental game is shown to be always higher than the one-shot optimal effort.

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VII-7

Time dependent mean-field games

Diogo A. Gomes, Edgard Pimentel and Héctor Sánchez-Morgado

We consider time dependent mean-field games (MFG) with a local power-like dependence on the measure and Hamiltonians satisfying both sub and superquadratic growth conditions. We establish existence of smooth solutions under a certain set of conditions depending both on the growth of the Hamiltonian as well as on the dimension. In the subquadratic case this is done by combining a Gagliardo-Nirenberg type of argument with a new class of polynomial estimates for solutions of the Fokker-Planck equation in terms of $L^r L^p$ norms of DpH. These techniques do not apply to the superquadratic case. In this setting we recur to a delicate argument that combines the non-linear adjoint method with polynomial estimates for solutions of the Fokker-Planck equation in terms of $L^\infty L^\infty$-norms of DpH. Concerning the subquadratic case, we substantially improve and extend the results previously obtained. Furthermore, to the best of our knowledge, the superquadratic case has not been addressed in the literature yet. In fact, it is likely that our estimates may also add to the current understanding of Hamilton-Jacobi equations with superquadratic Hamiltonians.

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VII-8

On Boundary feedback control of two-dimensional shallow flow

Ben Mansour Dia, Jesper Oppelstrup and Abdou Sene

We give an overview of different techniques to design local explicit feedback boundary conditions for the stabilization of the 2-D shallow water model around a given state. The first method uses domain decomposition and provides exponential decay of the energy. The second method is based on the symmetrization of the flux matrices and the analysis of the Riemann invariants. In the third part, we develop an algebraic Faedo-Galerkin technique to write stabilizing boundary conditions where the feedback control laws guarantee a decay of the defined energy. High order numerical simulations are performed to demonstrate how the proposed controllers work.

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VII-9

Discontinuos Galerkin approximations of hyperbolic problems

Blanca Ayuso de Dios and Saverio Castelanelli

We consider the application of the sparse grid technique for discontinuous Galerkin (DG) approximations of hyperbolic problems, with particular attention to the Vlasov-Poisson system. We describe the construction of the methods in the lowest order case and discuss their stability, error analysis and further properties. We include some simple numerical tests that show that the proposed sparse-grid DG method is indeed more efficient that the standard DG method, when comparing accuracy versus cost.

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VII-10

Size Estimates in Inverse Problems

Michele Di Cristo

Detection of inclusions or obstacles inside a body by boundary measurements is an inverse problems very useful in practical applications. When only finite numbers of measurements are available, we try to detect some information on the embedded object such as its size. In this talk we review some recent results on several inverse problems. The idea is to provide constructive upper and lower estimates of the area/volume of the unknown defect in terms of a quantity related to the work that can be expressed with the available boundary data.

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VII-11

An a Posteriori Error Estimate for Symplectic Euler Approximation of Optimal Control Problems

Mattias Sandberg, Jesper Karlsson, Stig Larsson, Anders Szepessy, Raúl Tempone

This work focuses on numerical solutions of optimal control problems. A time discretization error representation is derived for the approximation of the associated value function. It concerns Symplectic Euler solutions of the Hamiltonian system connected with the optimal control problem. The error representation has a leading order term consisting of an error density that is computable from Symplectic Euler solutions. Under an assumption of the pathwise convergence of the approximate dual function as the maximum time step goes to zero, we prove that the remainder is of higher order than the leading error density part in the error representation. With the error representation, it is possible to perform adaptive time stepping. We apply an adaptive algorithm originally developed for ordinary differential equations. The performance is illustrated by numerical tests.

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