



Advances in Uncertainty Quantification Methods, Algorithms and Applications (UQAW 2015)

January 6 – 9, 2015

9:00 a.m. – 5:00 p.m.

Level 0 auditorium, between Al-Jazri and Al-Kindi (buildings 4 and 5)

WORKSHOP TOPICS

- 1- Uncertainty Quantification Methods and Algorithms
- 2- Verification and Validation
- 3- Experimental Design
- 4- Applications to Problems in Computational Science, Engineering, Networks and the Environment

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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 3rd annual meeting of the Center, *Advances in Uncertainty Quantification Methods, Algorithms and Applications* (UQAW2015), January 6-9, 2015 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 third annual meeting is intended to report on the latest advances and innovations in Uncertainty Quantification Methods, Algorithms and Applications (UQAW 2015); 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 75 contributions (as oral or poster presentations) together with 20 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 2015, 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 2014

Raúl Tempone and Omar Knio

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	TUESDAY, JANUARY 6	WEDNESDAY, JANUARY 7	THURSDAY, JANUARY 8	FRIDAY, JANUARY 9	SATURDAY, JANUARY 10
8:30-9:00 a.m.	Breakfast		Breakfast	Breakfast	Local Meetings
9:00-9:30 a.m.	Welcome Registration	Center Presentation for Board Members only	Youssef Marzouk	Serge Prudhomme	
9:30-10:00 a.m.	Kody Law		Fabio Nobile	Quan Long	
10:00-10:30 a.m.	Hakan Bagci		Harald Haas	Oliver Ernst	
10:30-11:00 a.m.	Break	Slim Alouini	Break	Break	
11:00-11:30 a.m.	Raul Tempone	Ricardo Lima	Omar Ghattas	Mattias Sandberg	
11:30 a.m. - 12:00 p.m.		Fabrizio Bisetti		Ibrahim Hoteit	
12:00-1:30 p.m.	Lunch	Lunch	Lunch	Lunch	Lunch
1:30-2:00 p.m.	Olivier Le Maitre	Advisory Board Meeting	Advisory Board Meeting Follow-up	Advisory Board Report Presentation	Local Activities
2:00-2:30 p.m.	Alvaro Moraes				
2:30-3:00 p.m.	Break				
3:00-3:30 p.m.	Christian Bayer	Board Members Discussion	Board Members Discussion		
3:30-4:00 p.m.	Hermann Matthies	Matteo Icardi	Poster Session: University Library	Social activity: Economic City Beach	
4:00-4:30 p.m.	Poster set-up	Habib Najm			
5:00 p.m.	Welcome Reception: University Library				
6:00 p.m.		Conference Dinner: Al-Marsa Restaurant	Thuwal Dinner: Fish Restaurant	Economic City Dinner	

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Oral presentations

Perspectives on Nonlinear Filtering

Kody Law

The solution to the problem of nonlinear filtering may be given either as an estimate of the signal (and ideally some measure of concentration), or as a full posterior distribution. Similarly, one may evaluate the fidelity of the filter either by its ability to track the signal or its proximity to the posterior filtering distribution. Hence, the field enjoys a lively symbiosis between probability and control theory, and there are plenty of applications which benefit from algorithmic advances, from signal processing, to econometrics, to large-scale ocean, atmosphere, and climate modeling. This talk will survey some recent theoretical results involving accurate signal tracking with noise-free (degenerate) dynamics in high-dimensions (infinite, in principle, but say d between 10^3 and 10^8 , depending on the size of your application and your computer) [5, 1, 4, 3], and high-fidelity approximations of the filtering distribution in low dimensions (say d between 1 and several 10s) [6, 2].

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A Time Marching Scheme for Solving Volume Integral Equations on Nonlinear Scatterers

Hakan Bagci

Transient electromagnetic field interactions on inhomogeneous penetrable scatterers can be analyzed by solving time domain volume integral equations (TDVIEs). TDVIEs are oftentimes solved using marching-on-in-time (MOT) schemes. Unlike finite difference and finite element schemes, MOT-TDVIE solvers require discretization of only the scatterers, do not call for artificial absorbing boundary conditions, and are more robust to numerical phase dispersion. On the other hand, their computational cost is high, they suffer from late-time instabilities, and their implicit nature makes incorporation of nonlinear constitutive relations more difficult. Development of plane-wave time-domain (PWTD) and FFT-based schemes has significantly reduced the computational cost of the MOT-TDVIE solvers. Additionally, late-time instability problem has been alleviated for all practical purposes with the development of accurate integration schemes and specially designed temporal basis functions. Addressing the third challenge is the topic of this presentation.

I will talk about an explicit MOT scheme developed for solving the TDVIE on scatterers with nonlinear material properties. The proposed scheme separately discretizes the TDVIE and the nonlinear constitutive relation between electric field intensity and flux density. The unknown field intensity and flux density are expanded using half and full Schaubert-Wilton-Glisson (SWG) basis functions in space and polynomial temporal interpolators in time. The resulting coupled system of the discretized TDVIE and constitutive relation is integrated in time using an explicit $PE(CE)^m$ scheme to yield the unknown expansion coefficients. Explicitness of time marching allows for straightforward incorporation of the nonlinearity as a function evaluation on the right hand side of the coupled system of equations. Consequently, the resulting MOT scheme does not call for a Newton-like nonlinear solver. Numerical examples, which demonstrate the applicability of the proposed MOT scheme to analyzing electromagnetic interactions on Kerr-nonlinear scatterers will be presented.

Multi-Index Monte Carlo: when sparsity meets sampling

*Abdul-Lateef Haji-Ali, Fabio Nobile, and Raúl Tempone**

This talk focuses into our newest method: Multi Index Monte Carlo (MIMC). The MIMC method uses a stochastic combination technique to solve the given approximation problem, generalizing the notion of standard MLMC levels into a set of multi indices that should be properly chosen to exploit the available regularity. Indeed, instead of using first-order differences as in standard MLMC, MIMC uses high-order differences to reduce the variance of the hierarchical differences dramatically. This in turn gives a new improved complexity result that increases the domain of the problem parameters for which the method achieves the optimal convergence rate, $\mathcal{O}(\text{TOL}^{-2})$. Using optimal index sets that we determined, MIMC achieves a better rate for the computational complexity does not depend on the dimensionality of the underlying problem, up to logarithmic factors. We present numerical results related to a three dimensional PDE with random coefficients to substantiate some of the derived computational complexity rates. Finally, using the Lindeberg-Feller theorem, we also show the asymptotic normality of the statistical error in the MIMC estimator and justify in this way our error estimate that allows prescribing both the required accuracy and confidence in the final result.

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Polynomial Chaos Acceleration for the Bayesian Inference of Random Fields with Gaussian Priors and Uncertain Covariance Hyper-Parameters

Olivier Le Maitre, Ihab Sraj, Omar Knio and Ibrahim Hoteit*

We address model dimensionality reduction in the Bayesian inference of Gaussian fields, considering prior covariance function with unknown hyper-parameters. The Karhunen-Loeve (KL) expansion of a prior Gaussian process is traditionally derived assuming fixed covariance function with pre-assigned hyper-parameter values. Thus, the modes strengths of the Karhunen-Loeve expansion inferred using available observations, as well as the resulting inferred process, dependent on the pre-assigned values for the covariance hyper-parameters. Here, we seek to infer the process and its the covariance hyper-parameters in a single Bayesian inference. To this end, the uncertainty in the hyper-parameters is treated by means of a coordinate transformation, leading to a KL-type expansion on a fixed reference basis of spatial modes, but with random coordinates conditioned on the hyper-parameters. A Polynomial Chaos (PC) expansion of the model prediction is also introduced to accelerate the Bayesian inference and the sampling of the posterior distribution with MCMC method. The PC expansion of the model prediction also rely on a coordinates transformation, enabling us to avoid expanding the dependence of the prediction with respect to the covariance hyper-parameters. We demonstrate the efficiency of the proposed method on a transient diffusion equation by inferring spatially-varying log-diffusivity fields from noisy data.

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Hybrid Multilevel Monte Carlo Simulation of Stochastic Reaction Networks

Alvaro Moraes*, Raúl Tempone, Pedro Vilanova

Stochastic reaction networks (SRNs) is a class of continuous-time Markov chains intended to describe, from the kinetic point of view, the time-evolution of chemical systems in which molecules of different chemical species undergo a finite set of reaction channels.

This talk is based on articles [4, 5, 6], where we are interested in the following problem: given a SRN, X , defined through its set of reaction channels, and its initial state, x_0 , estimate $E(g(X(T)))$; that is, the expected value of a scalar observable, g , of the process, X , at a fixed time, T . This problem lead us to define a series of Monte Carlo estimators, $\mathcal{M}$, such that, with high probability can produce values close to the quantity of interest, $E(g(X(T)))$. More specifically, given a user-selected tolerance, TOL , and a small confidence level, η , find an estimator, $\mathcal{M}$, based on approximate sampled paths of X , such that,

$$P(|E(g(X(T))) - \mathcal{M}| \leq TOL) \geq 1 - \eta; \quad (1)$$

even more, we want to achieve this objective with near optimal computational work.

We first introduce a hybrid path-simulation scheme based on the well-known stochastic simulation algorithm (SSA)[3] and the tau-leap method [2]. Then, we introduce a Multilevel Monte Carlo strategy [1] that allows us to achieve a computational complexity of order $\mathcal{O}(TOL^{-2})$, this is the same computational complexity as in an exact method but with a smaller constant. We provide numerical examples to show our results.

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The forward-reverse method for conditional diffusion processes

Christian Bayer^{}, Alvaro Moraes, Raúl Tempone, Pedro Vilanova, John Schoenmakers and Hilmar Mai*

We derive stochastic representations for the finite dimensional distributions of a multidimensional diffusion on a fixed time interval, conditioned on the terminal state. The conditioning can be with respect to a fixed measurement point or more generally with respect to some subset. The representations rely on a reverse process connected with the given (forward) diffusion as introduced by Milstein, Schoenmakers and Spokoiny in the context of density estimation. The corresponding Monte Carlo estimators have essentially root-N accuracy, and hence they do not suffer from the curse of dimensionality. We also present an application in statistics, in the context of the EM algorithm.

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Non-Intrusive Solution of Stochastic and Parametric Equations

Hermann G. Matthies

Many problems depend on parameters, which may be a finite set of numerical values, or mathematically more complicated objects like for example processes or fields. We address the situation where we have an equation which depends on parameters; stochastic equations are a special case of such parametric problems where the parameters are elements from a probability space. One common way to represent this dependability on parameters is by evaluating the state (or solution) of the system under investigation for different values of the parameters. But often one wants to evaluate the solution quickly for a new set of parameters where it has not been sampled. In this situation it may be advantageous to express the parameter dependent solution with an approximation which allows for rapid evaluation of the solution. Such approximations are also called *proxy* or *surrogate models*, *response functions*, or *emulators*. All these methods may be seen as functional approximations—representations of the solution by an “easily computable” function of the parameters, as opposed to pure samples. The most obvious methods of approximation used are based on interpolation, in this context often labelled as collocation.

In the frequent situation where one has a “solver” for the equation for a given parameter value, i.e. a software component or a program, it is evident that this can be used to independently—if desired in parallel—solve for all the parameter values which subsequently may be used either for the interpolation or in the quadrature for the projection. Such methods are therefore uncoupled for each parameter value, and they additionally often carry the label “non-intrusive”. Without much argument all other methods—which produce a coupled system of equations—are almost always labelled as “intrusive”, meaning that one cannot use the original solver. We want to show here that this not necessarily the case.

Another approach is to choose some other projection onto the subspace spanned by the approximating functions. Usually this will involve minimising some norm of the difference between the true parametric solution and the approximation. Such methods are sometimes called *pseudo-spectral projections*, or *regression* solutions.

On the other hand, methods which try to ensure that the approximation satisfies the parametric equation as well as possible are often based on a Rayleigh-Ritz or Galerkin type of “ansatz”, which leads to a coupled system for the unknown coefficients. This is often taken as an indication that the original solver can not be used, i.e. that these methods are “intrusive”. But in many circumstances these methods may as well be used in a non-intrusive fashion. Some very effective new methods based on low-rank approximations fall in the class of “not obviously non-intrusive” methods; hence it is important to show here how this may be computed non-intrusively.

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Spectrum Scarcity and Optical Wireless Communications

Mohamed-Slim Alouini

Rapid increase in the use of wireless services over the last two decades has lead the problem of the radio-frequency (RF) spectrum exhaustion. More specifically, due to this RF spectrum scarcity, additional RF bandwidth allocation, as utilized in the recent past, is not anymore a viable solution to fulfill the demand for more wireless applications and higher data rates. Among the many proposed solutions, optical wireless communication or free-space optical (FSO) systems have gained an increasing interest due to their advantages including higher bandwidth and higher capacity compared to the traditional RF communication systems. This promising technology offers full-duplex Gigabit throughput in certain applications and environment while benefiting from a huge license-free spectrum, immunity to interference, and high security. These features of FSO communication systems potentially enable solving the issues that the RF communication systems face due to the expensive and scarce RF spectrum. The first part of the talk will give an overview of FSO communication systems by offering examples of advantages and application areas of this emerging technology. In the second part of talk, we will focus on some recent results and on-going research directions in the accurate characterization of the performance of FSO systems in the presence of inevitable impairments due to atmospheric turbulence and misalignment between transmitter and receiver.

Two-stage adaptive robust optimization of the Self-scheduling and Market Involvement for an Electricity Producer

Ricardo Manuel Pinto de Lima

This work address the optimization under uncertainty of the self-scheduling, forward contracting, and pool involvement of an electricity producer operating a mixed power generation station, which combines thermal, hydro and wind sources, and uses a two-stage adaptive robust optimization approach. In this problem the wind power production and the electricity pool price are considered to be uncertain, and are described by uncertainty convex sets. Two variants of a constraint generation algorithm are proposed, namely a primal and dual version, and they are used to solve two case studies based on two different producers. Their market strategies are investigated for three different scenarios, corresponding to as many instances of electricity price forecasts. The effect of the producers' approach, whether conservative or more risk prone, is also investigated by solving each instance for multiple values of the so-called budget parameter. It was possible to conclude that this parameter influences markedly the producers' strategy, in terms of scheduling, profit, forward contracting, and pool involvement. Regarding the computational results, these show that for some instances, the two variants of the algorithms have a similar performance, while for a particular subset of them one variant has a clear superiority.

Surrogate models and optimal design of experiments for chemical kinetics applications in combustion research

F. Bisetti, A. Farooq, D. Kim, O. Knio, Q. Long, R. Tempone*

Kinetic models for reactive flow applications comprise hundreds of reactions describing the complex interaction among many chemical species. The detailed knowledge of the reaction parameters is a key component of the design cycle of next-generation combustion devices, which aim at improving conversion efficiency and reducing pollutant emissions. Shock tubes are a laboratory scale experimental configuration, which is widely used for the study of reaction rate parameters.

Important uncertainties exist in the values of the thousands of parameters included in the most advanced kinetic models. This talk discusses the application of uncertainty quantification (UQ) methods to the analysis of shock tube data as well as the design of shock tube experiments. Attention is focused on a spectral framework in which uncertain inputs are parameterized in terms of canonical random variables, and quantities of interest (QoIs) are expressed in terms of a mean-square convergent series of orthogonal polynomials acting on these variables.

We outline the implementation of a recent spectral collocation approach for determining the unknown coefficients of the expansion, namely using a sparse, adaptive pseudo-spectral construction that enables us to obtain surrogates for the QoIs accurately and efficiently. We first discuss the utility of the resulting expressions in quantifying the sensitivity of QoIs to uncertain inputs, and in the Bayesian inference key physical parameters from experimental measurements.

We then discuss the application of these techniques to the analysis of shock-tube data and the optimal design of shock-tube experiments for two key reactions in combustion kinetics: the chain-branching reaction $\text{H} + \text{O}_2 \longleftrightarrow \text{OH} + \text{O}$ and the reaction of Furans with the hydroxyl radical OH.

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Multiphase flows in complex geometries: a UQ perspective

Matteo Icardi, Serge Prudhomme, Raúl Tempone*

Nowadays computer simulations are widely used in many multiphase flow applications involving interphases, dispersed particles, and complex geometries. Most of these problems are solved with mixed models composed of fundamental physical laws, rigorous mathematical upscaling, and empirical correlations/closures. This means that classical inference techniques or forward parametric studies, for example, becomes computationally prohibitive and must take into account the physical meaning and constraints of the equations. However mathematical techniques commonly used in Uncertainty Quantification can come to the aid for the (i) modeling, (ii) simulation, and (iii) validation steps. Two relevant applications for environmental, petroleum, and chemical engineering will be presented to highlight these aspects and the importance of bridging the gaps between engineering applications, computational physics and mathematical methods. The first example is related to the mathematical modeling of sub-grid/sub-scale information with Probability Density Function (PDF) models in problems involving flow, mixing, and reaction in random environment. After a short overview of the research field, some connections and similarities with Polynomial Chaos techniques, will be investigated. In the second example, averaged correlations laws and effective parameters for multiphase flow and their statistical fluctuations, will be considered and efficient computational techniques, borrowed from high-dimensional stochastic PDE problems, will be applied. In presence of interfacial flow, where small spatial scales and fast time scales are neglected, the assessment of robustness and predictive capabilities are studied. These illustrative examples are inspired by common problems arising, for example, from the modeling and simulation of turbulent and porous media flows.

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On Model Error and Statistical Calibration of Physical Models

Habib Najm

Existing methods for representation of model error in the statistical calibration of computational models typically rely on convolving model predictions of select observables with statistical data and model error terms. This strategy is successful in providing a statistical correction to model predictions in a manner that interpolates observations with meaningful uncertainty estimation between points. However, this approach faces a number of challenges when applied in the context of calibration of physical models, where, e.g. auxiliary physical constraints are in force, the model is intended for use outside the calibration regime, and other non-observable model output predictions are of interest.

We have developed a calibration strategy that addresses these challenges. We define constraints of interest as regards uncertain predictions, for example we require that the mean prediction is centered on the data, and that the predictive uncertainty is consistent with the range of discrepancy between the means of the prediction and the data. We embed statistical model error terms in select model components, where, e.g. specific phenomenological model assumptions are in force. We then formulate the problem as a density estimation problem and solve it using approximate Bayesian computation methods.

We demonstrate this construction on simple model problems, and for calibration of a simplified chemical model for methane-air kinetics against another, more complex, model. Select parameters of the simple model are encumbered by model error. We show how this uncertainty translates to model output uncertainty, and how the desired constraints on the uncertain prediction are achieved.

Transport maps for efficient Bayesian computation

Youssef Marzouk, Matthew Parno and Alessio Spantini*

We introduce a new framework for efficient sampling from complex probability distributions, using a combination of optimal transport maps and the Metropolis-Hastings rule. The core idea is to use continuous transportation to transform typical Metropolis proposal mechanisms (e.g., random walks, Langevin methods) into non-Gaussian proposal distributions that can more effectively explore the target density. Our approach adaptively constructs a lower triangular transport map—an approximation of the Knothe-Rosenblatt rearrangement—using information from previous MCMC states, via the solution of an optimization problem. This optimization problem is convex regardless of the form of the target distribution. It is solved efficiently using a Newton method that requires no gradient information from the target probability distribution; the target distribution is instead represented via samples. Sequential updates enable efficient and parallelizable adaptation of the map even for large numbers of samples. We show that this approach uses inexact or truncated maps to produce an adaptive MCMC algorithm that is ergodic for the exact target distribution. Numerical demonstrations on a range of parameter inference problems show order-of-magnitude speedups over standard MCMC techniques, measured by the number of effectively independent samples produced per target density evaluation and per unit of wallclock time.

We will also discuss adaptive methods for the construction of transport maps in high dimensions, where use of a non-adapted basis (e.g., a total order polynomial expansion) can become computationally prohibitive. If only samples of the target distribution, rather than density evaluations, are available, then we can construct high-dimensional transformations by composing sparsely parameterized transport maps with rotations of the parameter space. If evaluations of the target density and its gradients are available, then one can exploit the structure of the variational problem used for map construction. In both settings, we will show links to recent ideas for dimension reduction in inverse problems.

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Discrete least squares polynomial approximation with random evaluations – application to PDEs with random parameters

Giovanni Migliorati, Fabio Nobile, Raúl Tempone*

We consider a general problem $F(u, y) = 0$ where u is the unknown solution, possibly Hilbert space valued, and y a set of uncertain parameters. We specifically address the situation in which the parameter-to-solution map $u(y)$ is smooth, however y could be very high (or even infinite) dimensional. In particular, we are interested in cases in which F is a differential operator, u a Hilbert space valued function and y a distributed, space and/or time varying, random field.

We aim at reconstructing the parameter-to-solution map $u(y)$ from random noise-free or noisy observations in random points by discrete least squares on polynomial spaces. The noise-free case is relevant whenever the technique is used to construct metamodels, based on polynomial expansions, for the output of computer experiments. In the case of PDEs with random parameters, the metamodel is then used to approximate statistics of the output quantity.

We discuss the stability of discrete least squares on random points show convergence estimates both in expectation and probability. We also present possible strategies to select, either a-priori or by adaptive algorithms, sequences of approximating polynomial spaces that allow to reduce, and in some cases break, the curse of dimensionality.

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Li-Fi

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Networked visible light communications, also referred to as Li-Fi, promises quantum step improvements in area spectral efficiency while exploiting existing infrastructures by piggy-backing high speed data communication on existing lighting infrastructures. The visible light spectrum is unlicensed and 10,000 times larger than the range of radio frequencies between 0 Hz to 30 GHz. The use of the visible light spectrum for data communication is enabled by inexpensive and off-the-shelf available light emitting diodes (LEDs) which also form the basis for next generation energy efficient lighting. Individual LEDs can be modulated at very high speeds - 3.5 Gbit/s @ 2 m distance have been demonstrated as well as 1.1 Gbit/s @ 10m at the University of Edinburgh. Both demonstrations use micro LEDs with a total optical output power of 5 mW. LED lighting saves energy, and combining lighting and data communication adds additional energy saving benefits. Moreover, transforming the multiple light fixtures in a room into networked optical access points enables high density wireless networking referred to as optical attocell networks. While in radio frequency (RF) communication, multiple antennas as well as multiple transmission chains are required to achieve beamforming, this can simply be accomplished in Li-Fi by optical lenses. Because of this feature and the fact that light is spatially contained (and does not propagate through walls), effective interference management in high density optical attocell networks does not involve large computational complexity and very dense deployment of optical attocells is practically feasible. A by-product of the interference containment is enhanced security which could be exploited for new cybersecurity techniques. Recent research has shown that the area spectral efficiency indoors can be improved by a factor of 900 when using an optical attocell network. Thus it is possible to harness a vast and licence-free wireless transmission resource with existing devices; design optical access points to enable a new level of network densification without creating an unmanageable interference problem; thereby giving Li-Fi the capability to address jointly the issues of wireless data crunch, energy efficiency, security and simple transceivers for the large scale deployment of wireless devices.

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Bayesian Inversion for Large Scale Antarctic Ice Sheet Flow

Omar Ghattas*, Tobin Isaac, Noemi Petra, Georg Stadler

The flow of ice from the interior of polar ice sheets is the primary contributor to projected sea level rise. One of the main difficulties faced in modeling ice sheet flow is the uncertain spatially-varying Robin boundary condition that describes the resistance to sliding at the base of the ice. Satellite observations of the surface ice flow velocity, along with a model of ice as a creeping incompressible shear-thinning fluid, can be used to infer this uncertain basal boundary condition. We cast this ill-posed inverse problem in the framework of Bayesian inference, which allows us to infer not only the basal sliding parameters, but also the associated uncertainty. To overcome the prohibitive nature of Bayesian methods for large-scale inverse problems, we exploit the fact that, despite the large size of observational data, they typically provide only sparse information on model parameters. We show results for Bayesian inversion of the basal sliding parameter field for the full Antarctic continent, and demonstrate that the work required to solve the inverse problem, measured in number of forward (and adjoint) ice sheet model solves, is independent of the parameter and data dimensions.

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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.

Fast Bayesian optimal experimental design and its applications

Quan Long

We summarize our Laplace method and multilevel method of accelerating the computation of the expected information gain in a Bayesian Optimal Experimental Design (OED). Laplace method is a widely-used method to approximate an integration in statistics. We analyze this method in the context of optimal Bayesian experimental design and extend this method from the classical scenario, where a single dominant mode of the parameters can be completely-determined by the experiment, to the scenarios where a non-informative parametric manifold exists. We show that by carrying out this approximation the estimation of the expected Kullback-Leibler divergence can be significantly accelerated. While Laplace method requires a concentration of measure, multi-level Monte Carlo method can be used to tackle the problem when there is a lack of measure concentration. We show some initial results on this approach. The developed methodologies have been applied to various sensor deployment problems, e.g., impedance tomography and seismic source inversion.

Metropolis-Hastings Algorithms in Function Space for Bayesian Inverse Problems

Oliver G. Ernst, Björn Sprungk, Daniel Rudolf, Hans-Jörg Starkloff*

We consider Markov Chain Monte Carlo methods adapted to a Hilbert space setting. Such algorithms occur in Bayesian inverse problems where the solution is a probability measure on a function space according to which one would like to integrate or sample. We focus on Metropolis-Hastings algorithms and, in particular, we introduce and analyze a generalization of the existing pCN-proposal. This new proposal allows to exploit the geometry or anisotropy of the target measure which in turn might improve the statistical efficiency of the corresponding MCMC method. Numerical experiments for a real-world problem confirm the improvement.

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Computable error estimates for Monte Carlo finite element approximation of elliptic PDE with log normal diffusion coefficients

Eric Hall, Håkon Hoel, Mattias Sandberg, Anders Szepessy, Raúl Tempone*

The Monte Carlo (and Multi-level Monte Carlo) finite element method can be used to approximate observables of solutions to diffusion equations with log normal distributed diffusion coefficients, e.g. modelling ground water flow. Typical models use log normal diffusion coefficients with Hölder regularity of order up to $1/2$ a.s. This low regularity implies that the high frequency finite element approximation error (i.e. the error from frequencies larger than the mesh frequency) is not negligible and can be larger than the computable low frequency error. This talk will address how the total error can be estimated by the computable error.

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Targeted Sampling for Gaussian-Mixture Filtering High Dimensional Systems with Small Ensembles

Ibrahim Hoteit, Bo Lui, Dinh-Tuan Pham, Boujemaa Ait-El-Fquih, Mohamad El-Gharamti*

The update step of Gaussian-mixture filters consists of an ensemble of Kalman updates for each center of the mixture, generalizing the ensemble Kalman filters (EnKFs) update to non-Gaussian distributions. Sampling the posterior distribution is required to numerically integrate the posterior distribution forward with the dynamical model, which is known as the forecast step. Because of computational limitations, only small samples could be considered when dealing with large scale atmospheric and oceanic models. As such a "targeted" sampling that captures some features of the posterior distribution might be a better strategy than a straightforward random sampling. This was numerically demonstrated for the Gaussian-based ensemble filters, with the deterministic EnKFs outperforming the standard stochastic EnKF in many applications. In this talk, I will present two filtering algorithms based on this idea of "targeted" sampling; the first one introduces a deterministic sampling of the observational errors in the stochastic EnKF, and the second one is based on a Gaussian-mixture update step derived from a Kernel parameterization of the forecast sample and a resampling step matching the first two moments of the posterior. Numerical results with the popular Lorenz-96 model will be presented and discussed.

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Poster session I

Sampling methods and Stochastic processes

Multi-Index Monte Carlo: When Sparsity Meets Sampling

Abdul-Lateef Haji-Ali, Fabio Nobile, and Raúl Tempone

We propose and analyze a novel Multi-Index Monte Carlo (MIMC) method for weak approximation of stochastic models that are described in terms of differential equations either driven by random measures or with random coefficients. The MIMC method is both a stochastic version of the combination technique introduced by Zenger, Griebel and collaborators and an extension of the Multilevel Monte Carlo (MLMC) method first described by Heinrich and Giles. Inspired by Giles's seminal work, instead of using first-order differences as in MLMC, we use in MIMC high-order mixed differences to reduce the variance of the hierarchical differences dramatically. This in turn yields new and improved complexity results, which are natural generalizations of Giles's MLMC analysis, and which increase the domain of problem parameters for which we achieve the optimal convergence, $\mathcal{O}(\text{TOL}^{-2})$.

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Construction of a mean square error adaptive Euler–Maruyama method with applications in multilevel Monte Carlo

Håkon Hoel, Juho Häppölä, and Raúl Tempone

A formal mean square error expansion (MSE) is derived for Euler–Maruyama numerical solutions of stochastic differential equations (SDE). The error expansion is used to construct a pathwise *a posteriori* adaptive time stepping Euler–Maruyama method for numerical solutions of SDE, and the resulting method is incorporated into a multilevel Monte Carlo (MLMC) method for weak approximations of SDE. This gives an efficient MSE adaptive MLMC method for handling a number of low-regularity approximation problems. In low-regularity numerical example problems, the developed adaptive MLMC method is shown to outperform the uniform time stepping MLMC method by orders of magnitude, producing output whose error with high probability is bounded by $\text{TOL} > 0$ at the near-optimal cost rate $\mathcal{O}(\text{TOL}^{-2} \log(\text{TOL})^4)$.

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Flow, transport and diffusion in random geometries I: a MLMC algorithm

Claudio Canuto, Håkon Hoel, Matteo Icardi, Nathan Quadrio, Raúl Tempone

Multilevel Monte Carlo (MLMC) is an efficient and flexible solution for the propagation of uncertainties in complex models, where an explicit parametrization of the input randomness is not available or too expensive. We propose a general-purpose algorithm and computational code for the solution of Partial Differential Equations (PDEs) on random geometry and with random parameters. We make use of the key idea of MLMC, based on different discretization levels, extending it in a more general context, making use of a hierarchy of physical resolution scales, solvers, models and other numerical/geometrical discretization parameters. Modifications of the classical MLMC estimators are proposed to further reduce variance in cases where analytical convergence rates and asymptotic regimes are not available. Spheres, ellipsoids and general convex-shaped grains are placed randomly in the domain with different placing/packing algorithms and the effective properties of the heterogeneous medium are computed. These are, for example, effective diffusivities, conductivities, and reaction rates. The implementation of the Monte-Carlo estimators, the statistical samples and each single solver is done in parallel with a mixed parallelization approach.

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Error analysis in Fourier methods for option pricing for exponential Levy processes

Fabián Croce, Juho Häppölä, Jonas Kiessling and Raúl Tempone

We consider the Fourier method for european option pricing discussed by Carr Madan 1999 and then extended to more general processes and payoff by several authors. Assuming a Levy process for the log-price dynamics of the underlying asset, we deduce a bound for the error committed by the numerical method for a large class of payoff functions. The bound provided is simple to implement and to extend to new processes and payoffs. Furthermore, it provides a way of setting the parameters (damping, and cutoff) of the model to obtain the option price with maximum guaranteed accuracy. We provide examples showing how tight our bound is and how drastically the actual error can be reduced by a proper selection of the parameters.

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Hybrid Chernoff Tau-Leap

Alvaro Moraes, Raúl Tempone and Pedro Vilanova

Markovian pure jump processes can model many phenomena, e.g. chemical reactions at molecular level, protein transcription and translation, spread of epidemics diseases in small populations and in wireless communication networks among many others. In this work we present a novel hybrid algorithm for simulating individual trajectories which adaptively switches between the Stochastic Simulation Algorithm and the *Chernoff* Tau-leap Algorithm. This allows us to: (a) control the global exit probability of any simulated trajectory, (b) obtain accurate and computable estimates for the expected value of any smooth observable of the process with minimal computational work.

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Multilevel Hybrid Chernoff Tau-Leap

Alvaro Moraes, Raúl Tempone and Pedro Vilanova

Markovian pure jump processes can model many phenomena, e.g. chemical reactions at molecular level, protein transcription and translation, spread of epidemics diseases in small populations and in wireless communication networks, among many others. In this work, we present a novel Multilevel Monte Carlo algorithm based on our *Chernoff Hybrid Tau-leap* method for path-simulation of continuous time Markov pure jump processes. This multilevel approach can be viewed as a variance reduction technique that allows us to obtain accurate and computable estimates for the expected value of any smooth observable of the process with minimal computational work.

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Numerical Solution of Stochastic Nonlinear Fractional Differential Equations

Mohamed A. El-Beltagy and Amnah S. Al-Juhani

This work introduces a numerical estimation of the stochastic response of the Duffing oscillator with fractional or variable order damping and driven by white noise. The Wiener-Hermite expansion (WHE) with perturbation (WHEP) technique is integrated with the Grunwald-Letnikov approximation in case of fractional order and with Coimbra approximation in case of variable-order damping. The numerical solver was tested with the analytic solution and with Monte-Carlo simulations. The developed technique was shown to be efficient in simulating the stochastic differential equations with fractional or variable order derivatives.

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Computable error estimation for FEM for elliptic PDE with lognormal data

Eric Joseph Hall, Håkon Hoel, Mattias Sandberg, Anders Szepessy and Raúl Tempone

We derive computable error estimates for finite element approximations to elliptic PDE with *rough*, stochastic coefficients. In particular, we consider problems arising in subsurface flow where the coefficients are assumed to have a lognormal distribution. These estimators, based on local error indicators, are for observables of the pathwise Galerkin errors and of the expected quadrature errors committed in piecewise linear finite element approximations. Our theory is supported by numerical experiments for test problems in one and two dimensions.

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A Polynomial Chaos Expansion technique for correlated variables

Maria Navarro, Jeroen Witteveen and Joke Blom

In real-life problems, many situations exhibit correlations between model parameters. Those correlations have strong dynamical effects on the final solution, but many of the current uncertainty quantification (UQ) techniques do not take them into account. We propose a Polynomial Chaos Expansion (PCE) method for general multivariate distributions with correlated variables. The proposed method is as efficient as the original PCE: mean, variance and Sobol indices are computed without any extra computational cost and the convergence rate does not change. The method is illustrated with an application that shows how to propagate experimental errors through the process of fitting parameters to a probabilistic distribution of the quantities of interest. The application is also used to demonstrate the significant difference in the results assuming independence or full correlation compared to taking into account the true correlation.

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Poster session II

Low-rank and sparse approximation

II-1

Hierarchical matrix approximation of Matern covariance matrices

Alexander Litvinenko, Marc Genton and Ying Sun

The class of Matern covariance functions becomes very popular in spatial statistics and especially in geostatistics. We approximate large Matern covariance matrices in the hierarchical matrix format. We demonstrate a log-linear computational cost $\mathcal{O}(n \log n)$, where n is the number of points, of the matrix setup, matrix-vector product, matrix-matrix product, matrix-inversion and matrix update. All these operations can further allow to reduce the cost of e.g. Kriging or of the Kalman filter update. The matrix storage requirement is a log-linear as well. We demonstrate hierarchical matrix approximation of Matérn covariance functions for different smoothness parameters as well as for covariance lengths. To characterize the approximation error we will compute not only standard matrix norms, but also Kullback-Leibner divergence.

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II-2

Scalable Hierarchical Algorithms for stochastic PDEs and UQ

Alexander Litvinenko, Gustavo Chavez Chavez, David Keyes, Hatem Ltaief, Rio Yokota

KAUST SRI UQ Center started collaboration with KAUST Extreme Computing Research Center. There are few ideas which we will highlight. The first one is to extend/improve parallel implementation (R. Kriemann 2005, 2014) of hierarchical matrices [Hackbusch et al, 98] to the new hardware architecture: The Hierarchical matrix Computations on Multicore with hardware Accelerators (HiCMA) project aims to tackle the challenge that is facing the linear algebra community due to an unprecedented level of on-chip concurrency, introduced by the manycore era. HiCMA is a high performance numerical library designed for efficient compressions and fast implementations of ($\mathcal{H}$ -matrix) algorithms across a range of architectures: multicore, accelerators and ARM processors. The core idea is to redesign the numerical algorithms as implemented in $\mathcal{H}$ -Lib and to formulate them as successive calls to computational tasks, which are then scheduled on the underlying system using a dynamic runtime system to ensure load balancing. The algorithm is then represented as a Directed Acyclic Graph (DAG), where nodes represent tasks and edges show the data dependencies between them. There are various paramount factors such as admissibility condition (block partition), the minimal leaf size (diagonal block) and the $\mathcal{H}$ -matrix rank (numerical accuracy), which influence the performance of HiCMA. An auto-tuning framework is therefore critical to select the optimal parameters for a given application (FEM, BEM), which exhibits low rank matrix computations.

The second idea is to research how such factors as admissibility condition (i.e. block partition), the minimal leaf size (n_{min}) and the $\mathcal{H}$ -matrix rank influence on the efficiency of the parallel Hierarchical matrix implementation. Various admissibility conditions result in various block partitioning. We are looking for a partitioning which is more appropriate for the graphical Processor Units (GPUs) parallel architecture. To keep works on each processor balanced we are also trying to find an optimal relation between the minimal leaf size and the $\mathcal{H}$ -matrix rank.

A practical application of both ideas above is approximation of large covariance matrices which appears in statistical weather forecast in large regions (Europa, Saudi Arabia, Red Sea etc).

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II-3

Computation of the Response Surface in the Tensor Train data format

Alexander Litvinenko, Sergey Dolgov, Boris N. Khoromskij and Hermann G. Matthies

We apply the Tensor Train (TT) approximation to construct the Polynomial Chaos Expansion (PCE) of a random field, and solve the stochastic elliptic diffusion PDE with the stochastic Galerkin discretization. We compare two strategies of the polynomial chaos expansion: sparse and full polynomial (multi-index) sets. In the full set, the polynomial orders are chosen independently in each variable, which provides higher flexibility and accuracy. However, the total amount of degrees of freedom grows exponentially with the number of stochastic coordinates. To cope with this curse of dimensionality, the data is kept compressed in the TT decomposition, a recurrent low-rank factorization. PCE computations on sparse grids sets are extensively studied, but the TT representation for PCE is a novel approach that is investigated in this paper. We outline how to deduce the PCE from the covariance matrix, assemble the Galerkin operator, and evaluate some post-processing (mean, variance, Sobol indices), staying within the low-rank framework. The most demanding are two stages. First, we interpolate PCE coefficients in the TT format using a few number of samples, which is performed via the block cross approximation method. Second, we solve the discretized equation (large linear system) via the alternating minimal energy algorithm. In the numerical experiments we demonstrate that the full expansion set encapsulated in the TT format is indeed preferable in cases when high accuracy and high polynomial orders are required.

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Multilevel accelerated quadrature for PDEs with log-normal distributed random coefficient

Markus Siebenmorgen, Helmut Harbrecht, Michael Peters

We apply multilevel quadrature methods for the moment computation of the solution of stochastic partial differential equations with a log-normal distributed diffusion coefficient. The moment computation is a difficult task since they appear as high dimensional Bochner integrals on a unbounded integration domain. We are able to show convergence rates of classical quadrature methods for these Bochner integrals which are nearly independent of the dimensionality under certain regularity requirements on the stochastic input data. Each function evaluation in such a quadrature method corresponds to a deterministic elliptic boundary value problem which can be solved by e.g. finite elements on a fine enough discretization level. The complexity is therefore given by the number of quadrature points times the complexity for one elliptic PDE solve. The multilevel idea is to reduce this complexity by combining quadrature methods with different accuracies with several spatial discretization levels in a sparse grid like fashion. Hence, a quadrature formulas with high accuracy is used on the lowest spatial refinement level and quadrature formulas with lower accuracies are applied on the higher spatial refinement levels. Of course, this requires further regularity estimates of the solution. We present error and complexity estimates for the computation of the solution's first and second moment. Especially, the present framework covers the multilevel Monte Carlo method.

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Efficient approximation of random fields for numerical applications

Michael Peters, Helmut Harbrecht and Markus Siebenmorgen

We consider the rapid computation of separable expansions for the approximation of random fields. We compare approaches based on techniques from the approximation of non-local operators on the one hand and based on the pivoted Cholesky decomposition on the other hand. Especially, we provide an a-posteriori error estimate for the pivoted Cholesky decomposition in terms of the trace. Numerical examples are provided to validate and quantify the presented methods.

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II-6

Comparison of quasi-optimal and adaptive sparse grids for groundwater flow problems

Fabio Nobile, Lorenzo Tamellini, Raul Tempone, Francesco Tesei

In this work we consider a classical Darcy flow problem, in which the permeability field is modeled as a lognormal random field with tensorized Matérn covariance, i.e. a family of covariance functions depending on a scalar parameter ν that influences the smoothness of the corresponding realizations (with $\nu = \infty$ resulting in a random field with Gaussian covariance structure and $\nu = 0.5$ in an Exponential covariance, see e.g. [1]). In order to solve the Uncertainty Quantification problem (e.g. to estimate the mean and the variance of some quantity of interest related to the water flow), one first needs to introduce a finite-dimensional approximation of the permeability field, e.g. by a truncated Fourier or Karhunen–Loève expansion; however, for random fields with little regularity, a very high number of random variables will be needed to obtain a reasonable approximation of the permeability field, which renders the corresponding Uncertainty Quantification problem hard to tackle with methods like Stochastic Galerkin or Stochastic Collocation.

To overcome such difficulty, it is crucial to carefully exploit the intrinsic anisotropy of the problem, i.e. the fact that not all variables entering the approximation of the permeability field impact equally on the considered quantity of interest. In this work, we compare two possible approaches to this end: the “quasi-optimal” sparse grids that we have proposed in our previous works [2,3,4], and a generalization of the classical adaptive sparse grid algorithm by Gerstner and Griebel [5]. More precisely, the modifications that we have introduced allow to use non-nested quadrature points (in this case, Gauss–Hermite quadrature points), and to choose among different profit indicators that are suitable to drive the adaptation process.

In this poster we will present some preliminary results obtained for two different values of the smoothness parameter ν , i.e. $\nu = 2.5$ (that generates realizations of the log-permeability field which are twice differentiable) and $\nu = 0.5$ (whose corresponding log-permeability realizations are non-differentiable). Note that the second case has been made computationally tractable by applying to both the quasi-optimal and adaptive sparse grids schemes a single-level control variate approach, see [1]. The numerical results obtained suggest that the quasi-optimal and the adaptive sparse grid schemes perform comparably for both values of ν , and that moreover there is not a remarkable difference between sparse grids built with nested or non-nested points.

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Quasi-optimal sparse-grid approximations for random elliptic PDEs

Fabio Nobile, Lorenzo Tamellini, Raúl Tempone

Random differential equations 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 system at hand. 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 PDE solution u can be seen as a random function, $u = u(y_1, \dots, y_N)$, and usual goals include computing its mean and variance, or the probability that it exceeds a given threshold. Although this could be achieved with a straightforward Monte Carlo approach, such method may however be very demanding in terms of computational cost. Methods based on polynomial approximations of $u(y_1, \dots, y_N)$ have thus been introduced, aiming at exploiting the possible regularity of u with respect to $y_1, \dots, y_N$ to alleviate the computational burden. These 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, such 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 . More precisely, 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.

This method is very general and can be used to build sparse grids either on bounded or unbounded domains (e.g. uniform and normal random distributions for y_n), using both nested and non-nested families of univariate collocation points (e.g. Clenshaw–Curtis, Leja, Genz–Keister, Gauss–Legendre or Gauss–Hermite points). We will present some theoretical convergence results as well as numerical results showing the efficiency of the proposed approach for the above-mentioned cases.

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Goal-Oriented Compression of Random Fields

Ingolf Busch, Oliver G. Ernst, and Björn Sprungk Raúl Tempone

We consider expansions of the input random field of a diffusion equation with respect to a set of L^2 -orthogonal functions. The objective is to find such a compressed expansion which is adapted to a given quantity of interest, which is a functional of the random PDE solution. Our method uses a combination of variational and sampling techniques. Preliminary results indicate possible gains versus the standard KL expansion of the input field when the quantity of interest is sufficiently localized.

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Poster session III
Bayesian Inference and Filtering

III-1

Dimension-independent likelihood-informed MCMC samplers

Tiangang Cui, Kody J.H. Law, and Youssef Marzouk

Many Bayesian inference problems require exploring the posterior distribution of high-dimensional parameters, which in principle can be described as functions. By exploiting low-dimensional structure in the change from prior to posterior [distributions], we introduce a suite of MCMC samplers that can adapt to the complex structure of the posterior distribution, yet are well-defined on function space. Posterior sampling in nonlinear inverse problems arising from various partial differential equations and also a stochastic differential equation are used to demonstrate the efficiency of these dimension-independent likelihood-informed samplers.

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III-2

Multi-level ensemble Kalman filter

Håkon Hoel, Kody J.H. Law, and Raúl Tempone

This work embeds a multi-level monte-carlo (MLMC) sampling strategy into the monte-carlo step of the ensemble Kalman filter (ENKF), thereby yielding a multi-level ensemble Kalman filter (MLENKF) which has provably superior asymptotic cost to a given accuracy level. The theoretical results are illustrated numerically.

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III-3

Evaluating Data Assimilation Algorithms

Kody J.H. Law, and Andrew M. Stuart

Data assimilation leads naturally to a Bayesian formulation in which the posterior probability distribution of the system state, given the observations, plays a central conceptual role. The aim of this paper is to use this Bayesian posterior probability distribution as a gold standard against which to evaluate various commonly used data assimilation algorithms. A key aspect of geophysical data assimilation is the high dimensionality and low predictability of the computational model. With this in mind, yet with the goal of allowing an explicit and accurate computation of the posterior distribution, we study the 2D Navier-Stokes equations in a periodic geometry. We compute the posterior probability distribution by state-of-the-art statistical sampling techniques. The commonly used algorithms that we evaluate against this accurate gold standard, as quantified by comparing the relative error in reproducing its moments, are 4DVAR and a variety of sequential filtering approximations based on 3DVAR and on extended and ensemble Kalman filters. The primary conclusions are that: (i) with appropriate parameter choices, approximate filters can perform well in reproducing the mean of the desired probability distribution; (ii) however they typically perform poorly when attempting to reproduce the covariance; (iii) this poor performance is compounded by the need to modify the covariance, in order to induce stability. Thus, whilst filters can be a useful tool in predicting mean behavior, they should be viewed with caution as predictors of uncertainty. These conclusions are intrinsic to the algorithms and will not change if the model complexity is increased, for example by employing a smaller viscosity, or by using a detailed NWP model.

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III-4

Mean-field ensemble Kalman filtering

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Filtering of a continuous-time stochastic process which is observed at discrete observation times is considered. A generalized ensemble Kalman filter (EnKF) is introduced which extends the classical EnKF algorithm from Gaussian state-space models to non-Gaussian state-space models with Gaussian observations. The latter arises for example in the case that the hidden continuous-time stochastic process has a nonlinear drift and is observed discretely in time. A recursion for the density of the mean-field limit of this EnKF algorithm is derived. A method is proposed in which an accurate numerical approximation of the Fokker-Planck equation is used to obtain the predicting density. A quadrature rule is then used to approximate either (a) the true filtering density arising from Bayesian analysis, (b) the mean-field EnKF density, or (c) a Gaussian approximation. The local error of the EnKF is bounded by the sum of two components: (i) the error between the finite approximation and the mean-field limit (sample or discretization error), and (ii) the error between the mean-field limit and the true filtering distribution (linear update error). In its simplest form presented here we show that under suitable assumptions the error (i) is asymptotically smaller using this new approach as compared to standard EnKF for sufficiently low model dimensions, and therefore either of (a,b,c) outperform standard EnKF as long as (i) is the dominant source of error. Once error (ii) exceeds error (i) this improvement is irrelevant and standard EnKF with any sufficiently large ensemble size is comparable to (b). Numerical experiments are performed for both a linear and a nonlinear Langevin SDE in order to confirm the theoretical results and further investigate the effects of error (ii). In the nonlinear case, we examine the effect of imposing a Gaussian approximation on the distribution and find that the approximate Gaussian filter may perform better than the non-Gaussian mean-field EnKF, depending on when the Gaussian approximation is imposed. These results can be used to develop more effective filters.

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III-5

Bayesian Optimal Experimental Design Using Multilevel Monte Carlo

Chaouki ben Issaid, Quan Long, Marco Scavino and Raúl Tempone

Experimental design is very important since experiments are often resource-exhaustive and time-consuming.

We carry out experimental design in the Bayesian framework.

To measure the amount of information, which can be extracted from the data in an experiment, we use the expected information gain as the utility function, which specifically is the expected logarithmic ratio between the posterior and prior distributions. Optimizing this utility function enables us to design experiments that yield the most informative data for our purpose. One of the major difficulties in evaluating the expected information gain is that the integral is nested and can be high dimensional. We propose using multilevel Monte Carlo techniques to accelerate the computation of the nested high dimensional integral. The advantages are two-fold. First, the multilevel Monte Carlo can significantly reduce the cost of the nested integral for a given tolerance, by using an optimal sample distribution among different sample averages of the inner integrals. Second, the multi level Monte Carlo method imposes less assumptions, such as the concentration of measures, required by Laplace method. We test our multi level Monte Carlo technique using a numerical example on the design of sensor deployment for a Darcy flow problem governed by one dimensional Laplace equation. We also compare the performance of the multi level Monte Carlo, Laplace approximation and direct double loop Monte Carlo.

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III-6

Bayesian Inference for Linear Parabolic PDEs with Noisy Boundary Conditions

Fabrizio Ruggeri, Zaid Sawlan, Marco Scavino and Raúl Tempone

In this work we develop a hierarchical Bayesian setting to infer unknown parameters in initial-boundary value problems (IBVPs) for one-dimensional linear parabolic partial differential equations. Noisy boundary data and known initial condition are assumed. We derive the likelihood function associated with the forward problem, given some measurements of the solution field subject to Gaussian noise. Such function is then analytically marginalized using the linearity of the approximated solution of the forward problem. Gaussian priors have been assumed for the time-dependent Dirichlet boundary values. Our approach is applied to synthetic data for the one-dimensional heat equation model, where the thermal diffusivity is the unknown parameter. We show how to infer the thermal diffusivity parameter when its prior distribution is lognormal or modeled by means of a space-dependent stationary lognormal random field. We use the Laplace method to provide approximated Gaussian posterior distributions for the thermal diffusivity. Expected information gains and predictive posterior densities for observable quantities are numerically estimated for different experimental setups.

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III-7

Fast Bayesian Optimal Experimental Design for Seismic Source Inversion

Quan Long, Mohammad Motamed and Raúl Tempone

We develop a fast method for optimally designing experiments in the context of statistical seismic source inversion. In particular, we efficiently compute the optimal number and locations of the receivers or seismographs. The seismic source is modeled by a point moment tensor multiplied by a time-dependent function. The parameters include the source location, moment tensor components, and start time and frequency in the time function. The forward problem is modeled by elastodynamic wave equations. We show that the Hessian of the cost functional, which is usually defined as the square of the weighted L_2 norm of the difference between the experimental data and the simulated data, is proportional to the measurement time and the number of receivers. Consequently, the posterior distribution of the parameters, in a Bayesian setting, concentrates around the “true” parameters, and we can employ Laplace approximation and speed up the estimation of the expected Kullback-Leibler divergence (expected information gain), the optimality criterion in the experimental design procedure. Since the source parameters span several magnitudes, we use a scaling matrix for efficient control of the conditional number of the original Hessian matrix. We use a second-order accurate finite difference method to compute the Hessian matrix and either sparse quadrature or Monte Carlo sampling to carry out numerical integration. We demonstrate the efficiency, accuracy, and applicability of our method on a two-dimensional seismic source inversion problem.

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III-8

Minimum mean square error estimation and approximation of the Bayesian update

Alexander Litvinenko, Elmar Zander and Hermann G. Matthies

The Bayesian Update (BU) 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 non-linear extension of the well-known Kalman filter, which we call non-linear Bayesian update (NLBU). We derive it from the minimum mean square error estimation. The idea is to get the update formula for all Polynomial Chaos coefficients and not only for the mean and covariance. We demonstrate two examples: elliptic PDE with uncertain permeability coefficient and a chaotic Lorenz 84 model with random coefficients.

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III-9

Adaptive Surrogate Modeling for Response Surface Approximations with Application to Bayesian Inference

Serge Prudhomme and Corey M. Bryant

The need for surrogate models and adaptive methods can be best appreciated if one is interested in parameter estimation using a Bayesian calibration procedure for validation purposes [1,2]. We extend here our latest work on error decomposition and adaptive refinement for response surfaces [3] to the development of surrogate models that can be substituted for the full models to estimate the parameters of Reynolds-averaged Navier-Stokes models. The error estimates and adaptive schemes are driven here by a quantity of interest and are thus based on the approximation of an adjoint problem. We will focus in particular to the accurate estimation of evidences to facilitate model selection. The methodology will be illustrated on the Spalart-Allmaras RANS model for turbulence simulation.

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Seismic data assisted history matching using ensemble based methods for the Norne Field in Norway - A real field study

Klemens Katterbauer, Santiago Arango, Shuyu Sun, Ibrahim Hoteit

The Norne Field is a large reservoir structure in the northern part of offshore North Sea and was successfully discovered in 1992 and put on production in 1997. Considerable extraction from the reservoir led to a significant depletion of the reservoir formation and formation pressure drop that was partially sustained by water injection. With the rapid depletion of the reservoir, Statoil was focusing on better characterizing the reservoir to determine water-infiltrated sections and optimize their field development plans. During the course of production, time lapse seismic surveys were collected for monitoring the dynamics in the reservoir and these data were integrated into an ensemble based history matching framework for matching the production data from the reservoir and incorporate the correlation effects of the seismic data to the water saturation to detect better water saturation levels. The study outlines the feasibility of the integration of seismic data for real field applications to enhance reservoir forecasts and quantify uncertainty.

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The Forward-Reverse Algorithm for Stochastic Reaction Networks with Applications to Statistical Inference

Alvaro Moraes¹, Christian Bayer², Raúl Tempone¹ and Pedro Vilanova¹

In this work, we present an extension of the forward-reverse algorithm by Bayer and Schoenmakers [Annals of Applied Probability, 24(5):1994–2032, October 2014] to the context of stochastic reaction networks (SRNs). It makes the approximation of expected values of functionals of bridges for this type of processes computationally feasible. We then apply this bridge-generation technique to the statistical inference problem of approximating the reaction coefficients based on discretely observed data. To this end, we introduce a two-phase iterative inference method in which, starting from a set of over-dispersed initial guesses, we solve a set of deterministic optimization problems where the SRNs are replaced by the classical ODE rates; then, during the second phase, the Monte Carlo version of the EM algorithm is applied starting from the outputs of the previous phase. The output of our two-phase method is a cluster of maximum likelihood estimates obtained by using convergence assessment techniques from the theory of Markov chain Monte Carlo. Our results are illustrated by numerical examples.

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Poster session IV
Green Wireless Communication

IV-1

Energy-Efficient Power Allocation of Cognitive Radio Systems without CSI at the Transmitter

Lokman Sboui, Zouheir Rezki, and Mohamed-Slim Alouini

Within the growing demand for wireless communications, a major challenge is to improve the energy efficiency (EE) of future systems and reduce the CO₂ emission. In this context, we present a power allocation framework for spectrum sharing Cognitive Radio (CR) systems based on maximizing the EE. We, first, derive an explicit expression of the optimal power with instantaneous channel gain based on EE criterion for a single user system. We also solve a non-convex problem and compute explicitly the optimal power for ergodic EE under either a peak or an average power constraint. When the instantaneous channel is not available, we provide the optimal power equation and compute simple sub-optimal power. Afterwards, we apply our results on underlay cognitive radio (CR) systems where the power is limited by an additional interference constraint. In the numerical results, we show that the sub-optimal solution is very close to the optimal solution. We, also, show that the absence of the channel state information (CSI) only affects the EE performances at high power regime. In the CR context, we show that the interference threshold has a minimal effect on the EE compared to the spectral efficiency.

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IV-2

A Game Theoretical Approach for Cooperative Environmentally Friendly Cellular Networks Powered by the Smart Grid

Hakim Ghazzai, Elias Yaacoub, Mohamed-Slim Alouini

This paper investigates the collaboration between multiple mobile operators to optimize the energy efficiency of cellular networks, maximize their profits or achieve a tradeoff between both objectives. Mobile operators cooperate together by eliminating redundant base stations (BSs) using a low complexity algorithm that aims to maximize their objective functions subject to a quality of service constraint. The problem is modeled as a two-level Stackelberg game: a mobile operator level and a smart grid level. Indeed, in our framework, we assume that cellular networks are powered by multiple energy providers existing in the smart grid characterized by different pollutant levels in addition to renewable energy source deployed in BS sites. The objective is to find the best active BS combination and the optimal procurement decision needed to the network operation during collaboration by considering electricity real-time pricing. Our study includes the daily traffic variation in addition to the daily green energy availability. Our simulation results show a significant saving in terms of CO₂ emissions compared to the non-collaboration case and that cooperative mobile operators exploiting renewables are more awarded than traditional operators.

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IV-3

On the Symbol Error Rate of M-ary MPSK over Generalized Fading Channels with Additive Laplacian Noise

Hamza Soury and Mohamed-Slim Alouini

This paper considers the symbol error rate of M-ary phase shift keying (MPSK) constellations over extended Generalized-K fading with Laplacian noise and using a minimum distance detector. A generic closed form expression of the conditional and the average probability of error is obtained and simplified in terms of the Fox's H function. More simplifications to well known functions for some special cases of fading are also presented. Finally, the mathematical formalism is validated with some numerical results examples done by computer based simulations.

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Energy-Aware Amplify-and-Forward Relaying Systems with Imperfect Channel Estimation

Osama Amin, Ebrahim Bedeer, Mohamed H. Ahmed, Octavia A. Dobre, and Mohamed-Slim Alouini

The green design of wireless communication systems uses the energy efficiency (EE) metric that should capture all energy consumption sources to deliver the required data. In this research, we formulate an accurate EE metric for two-hop amplify-and-forward relaying systems that considers the impact of channel estimation. Two channel estimation strategies are assumed namely disintegrated channel estimation, which assumes the availability of channel estimator at the relay, and cascaded channel estimation, where the relay is not equipped with channel estimator and only forwards the received pilot(s) in order to let the destination estimate the cooperative link. The channel estimation cost is reflected on the EE metric by including the estimation error in the signal-to-noise ratio in the achievable rate term and considering the energy consumption during the channel estimation phase. The estimated channel state information is used to optimally allocate the power of both the source and the relay to maximize the proposed EE metric. Moreover, we investigate the effect of the estimation parameters on the optimized EE performance through simulation examples.

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Fully-distributed randomized cooperation in wireless sensor networks

Ahmed Bader, Karim Abed-Meraim, and Mohamed-Slim Alouini

When marrying randomized distributed space-time coding (RDSTC) to geographical routing, new performance horizons can be created. In order to reach those horizons however, routing protocols must evolve to operate in a fully distributed fashion. In this letter, we expose a technique to construct a fully distributed geographical routing scheme in conjunction with RDSTC. We then demonstrate the performance gains of this novel scheme by comparing it to one of the prominent classical schemes.

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An Efficient Simulation Method for Rare Events

Madhir Ben Rached, Fatma Benkhelifa, Abba Kammoun, Mohamed-Slim Alouini, and Raúl Tempone

Estimating the probability that a sum of random variables (RVs) exceeds a given threshold is a well-known challenging problem. Closed-form expression of the sum distribution is usually intractable and presents an open problem. A crude Monte Carlo (MC) simulation is the standard technique for the estimation of this type of probability. However, this approach is computationally expensive especially when dealing with rare events (i.e events with very small probabilities). Importance Sampling (IS) is an alternative approach which effectively improves the computational efficiency of the MC simulation. We develop a general framework based on IS approach for the efficient estimation of the probability that the sum of independent and not necessarily identically distributed any RVs exceeds a given threshold. The proposed IS approach is based on constructing a new sampling distribution by twisting the hazard rate of the original underlying distribution of each component in the summation. A minmax approach is carried out for the determination of the twisting parameter, for any given threshold. Moreover, using this minmax optimal choice, the estimation of the probability of interest is shown to be asymptotically optimal as the threshold goes to infinity. We also offer some selected simulation results illustrating first the efficiency of the proposed IS approach. The near-optimality of the minmax approach is then numerically analyzed.

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Power Efficient Low Complexity Precoding for Massive MIMO Systems

Houssem Sifaou, Abba Kammoun, Luca Sanguinetti Mérouane Debbah and Mohamed-Slim Alouini

This work aims at designing a low-complexity precoding technique in the downlink of a large-scale multiple-input multiple-output (MIMO) system in which the base station (BS) is equipped with M antennas to serve K single-antenna user equipments. This is motivated by the high computational complexity required by the widely used zero-forcing or regularized zero-forcing precoding techniques, especially when K grows large. To reduce the computational burden, we adopt a precoding technique based on truncated polynomial expansion (TPE) and make use of the asymptotic analysis to compute the deterministic equivalents of its corresponding signal-to-interference-plus-noise ratios (SINRs) and transmit power. The asymptotic analysis is conducted in the regime in which M and K tend to infinity with the same pace under the assumption that imperfect channel state information is available at the BS. The results are then used to compute the TPE weights that minimize the asymptotic transmit power while meeting a set of target SINR constraints. Numerical simulations are used to validate the theoretical analysis.

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Performance Limits of Energy Harvesting Communications under Imperfect Channel State Information

Mohamed Ridha Zenaidi, Zouheir Rezki, Hamidou Tembine and Mohamed-Slim Alouini

In energy harvesting communications, the transmitters have to adapt transmission to availability of energy harvested during the course of communication. The performance of the transmission depends on the channel conditions which vary randomly due to mobility and environmental changes. In this work, we consider the problem of power allocation taking into account the energy arrivals over time and the degree of channel state information (CSI) available at the transmitter, in order to maximize the throughput. Differently from other works, the CSI at the transmitter is not perfect and may include estimation errors. We solve this problem with respect to the causality and energy storage constraints. We determine the optimal offline policy in the case where the channel is assumed to be perfectly known at the receiver. Different cases of CSI availability are studied for the transmitter. We obtain the power policy when the transmitter has either perfect CSI or no CSI. We also investigate of utmost interest the case of fading channels with imperfect CSI. Furthermore, we analyze the asymptotic average throughput in a system where the average recharge rate goes asymptotically to zero and when it is very high.

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Low Complexity Beampattern Design in MIMO Radars Using Planar Array

Taha Bouchoucha, Sajid Ahmed, Tareq Al-Naffouri and Mohamed-Slim Alouini

In multiple-input multiple-output radar systems, it is usually desirable to steer transmitted power in the region-of-interest. To do this, conventional methods optimize the waveform covariance matrix, $\mathbf{R}$, for the desired beampattern, which is then used to generate actual transmitted waveforms. Both steps require constrained optimization, therefore, use iterative and expensive algorithms. In this paper, we provide a closed-form solution to design covariance matrix for the given beampattern using the planar array, which is then used to derive a novel closed-form algorithm to directly design the finite-alphabet constant-envelope (FACE) waveforms. The proposed algorithm exploits the two-dimensional fast-Fourier-transform. The performance of our proposed algorithm is compared with existing methods that are based on semi-definite quadratic programming with the advantage of a considerably reduced complexity.

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Secret-Sharing over Multiple-Antenna Channels with Transmit Correlation

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We consider secret-key agreement with public discussion over Rayleigh fast-fading channels with transmit correlation. The legitimate receiver and the eavesdropper are assumed to have perfect channel knowledge while the transmitter has only knowledge of the transmit correlation matrix. First, We derive the expression of the key capacity under the considered setup. Then, we show that the optimal transmit strategy achieving the key capacity consists in transmitting Gaussian signals along the eigenvectors of the channel covariance matrix. The powers allocated to each channel mode are determined as the solution of a numerical optimization problem that we derive. We also provide a waterfilling interpretation of the optimal power allocation. Finally, we develop a necessary and sufficient condition for beamforming to be optimal, i.e., transmitting along the strongest channel mode only is key capacity-achieving.

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Poster session V
Computational Electro-Magnetics

Sparse Electromagnetic Imaging using Nonlinear Landweber Iterations

Abdulla Desmal and Hakan Bağcı

A nonlinear optimization scheme for electromagnetic imaging of sparse domains is described. The proposed method, unlike previously developed schemes, does not rely on an implicitly- or explicitly-enforced linearization of the scattering operator but directly uses a nonlinear Tikhonov-based approach. This approach constructs the nonlinear least-squares problem for the data misfit between measured scattered fields and those formulated as a nonlinear function of domain's complex permittivity. The resulting minimization problem in unknown permittivity is solved using nonlinear Landweber iterations. The sparsity constraint is enforced by applying a thresholding function at every iteration. Additionally, a frequency hopping scheme is proposed to account for multiple-frequency measurements within the thresholded nonlinear Landweber iterations. Numerical experiments, which make use of synthetically and experimentally generated data, demonstrate the accuracy and efficiency of the proposed inversion algorithm.

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Analysis of Electromagnetic Wave Interactions on Nonlinear Scatterers using Time Domain Volume Integral Equations

Hüseyin Arda Ülkü, Sadeed Bin Sayed, and Hakan Bağcı

An explicit marching on in time (MOT) scheme for characterizing electromagnetic wave interactions on scatterers with nonlinear material properties is described. The proposed scheme separately discretizes the time domain electric field volume integral equation (TDVIE) and the nonlinear constitutive relation between electric field intensity and flux density. The unknown field intensity and flux density are expanded using half and full Schaubert-Wilton-Glisson basis functions in space and polynomial temporal interpolators in time. The resulting coupled system of the discretized TDVIE and constitutive relation is integrated in time using an explicit $PE(CE)^m$ scheme to yield the unknown expansion coefficients. Explicitness of time marching allows for straightforward incorporation of the nonlinearity as a function evaluation on the right hand side of the coupled system of equations. Consequently, the resulting MOT scheme does not call for a Newton-like nonlinear solver. Numerical examples, which demonstrate the applicability of the proposed MOT scheme to analyzing electromagnetic interactions on Kerr-nonlinear scatterers are presented.

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An Efficient Explicit Time Marching Scheme for Solving the Time Domain Magnetic Field Volume Integral Equation

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Transient electromagnetic scattering from inhomogeneous dielectric objects can be analyzed by solving time domain volume integral equations (TDVIEs). TDVIE solvers discretize unknown currents/fields using spatial basis functions and temporal interpolators. This leads to a system of equations that can be solved via a marching on in time (MOT) scheme. Depending on the type of spatial and temporal interpolators, the resulting MOT scheme can be implicit (N. T. Gres, *et al.*, *Radio Sci.*, 36(3), 379-386, 2001) or explicit (A. Al-Jarro, *et al.*, *IEEE Trans. Antennas Propag.*, 60(11), 5203-5214, 2012). Though more stable and accurate, implicit MOT solvers are less efficient for low frequency problems since they call for inversion of a full matrix at every time step. On the other hand, explicit MOT solvers are less stable and call for smaller time steps to guarantee a stable and accurate solution. In this work, the explicit MOT scheme originally developed for solving the time domain surface magnetic field integral equation (H. A. Ulku, *et al.*, *IEEE Trans. Antennas Propag.*, 61(8), 4120-4131, 2013) is extended to solving the time domain magnetic field volume integral equation (TDMFVIE). The proposed solver expands the magnetic field inside the dielectric scatterer using first order curl-conforming spatial basis functions and polynomial temporal interpolators. Using this expansion and applying point testing, a semi-discrete system of equations is obtained. This system is integrated in time using a predictor corrector scheme (A. Glaser and V. Rokhlin, *J. Sci. Comput.*, 38(3), 368-399, 2009) to find the unknown expansion coefficients. The resulting MOT solver combines the advantages of previously developed explicit and implicit solvers:

- (i) It does not require a matrix inversion and is faster than the implicit solvers for low frequency problems.
- (ii) The time step size is as large as those of the implicit solvers without sacrificing accuracy or stability.

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A Novel Time Domain Method for Characterizing Plasmonic Field Interactions

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A time domain surface integral equation (TD-SIE) solver for analyzing transient plasmonic interactions on nanostructures is described. The proposed solver makes use of the Poggio-Miller-Chan-Harrington-Wu-Tsai (PMCHWT) SIE formulation to construct the scattered fields in the form of a spatio-temporal convolution of equivalent surface electric and magnetic current densities, which are introduced at material interfaces, with the Green function of the unbounded dispersive medium. Equivalent currents are expanded using 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 discrete time steps yield a matrix system of equations. The samples of the time domain Green function required by this process to compute the matrix entries are obtained from frequency domain samples using a fast relaxed vector fitting (FRVF) algorithm. This matrix system of equations then is solved for the unknown expansion coefficients using a marching on in time (MOT) scheme. Numerical results, which demonstrate the applicability and accuracy of the proposed MOT-TD-PMCHWT-SIE solver, are presented.

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Analysis of Transient Electromagnetic Wave Interactions on Graphene Sheets Using Integral Equations

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A marching on in time (MOT) scheme for analyzing transient electromagnetic wave interactions on thin graphene sheets is described. The proposed scheme discretizes a time domain resistive boundary condition (TDRBC) enforced on the graphene sheet that is assumed infinitesimally thin. The unknown current density induced on this surface is expanded using Rao-Wilton-Glisson (RWG) functions in space and polynomial interpolants in time. Inserting this expansion into the TDRBC and Galerkin-testing the resulting equation at discrete time steps yield a matrix system of equations. The samples of graphene's conductivity required by this process to compute the matrix entries are obtained from frequency domain samples using a fast relaxed vector fitting (FRVF) algorithm. This time-domain integral-equation based approach avoids generation of volumetric meshes with high aspect ratios that would otherwise be required by finite-element and finite-difference based methods. Numerical results demonstrating the benefits of the proposed scheme are presented.

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A Hybrid DGTD-MNA Scheme for Analyzing Complex Electromagnetic Systems

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A hybrid electromagnetics (EM)-circuit simulator for analyzing complex systems consisting of microwave devices loaded with nonlinear multi-port lumped circuits is described. The proposed scheme splits the computation domain into two: EM and circuit subsystems, where field interactions are modeled using Maxwell and Kirchhoff equations, respectively. Maxwell equations are discretized using a discontinuous Galerkin time domain (DGTD) scheme while Kirchhoff equations are discretized using a modified nodal analysis (MNA)-based scheme. The coupling between the EM and circuit subsystems is realized at the lumped ports, where related EM fields and port voltages and currents are allowed to “interact” via numerical flux. To account for nonlinear lumped circuit elements, the standard Newton-Raphson method is applied at every time step. Additionally, a local time-stepping scheme is developed to improve the efficiency of the hybrid solver. Numerical examples including microwave devices loaded with single and multiport linear/nonlinear circuit networks are presented to demonstrate the accuracy, efficiency, and applicability of the proposed solver.

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Efficient Computation of Electromagnetic Fields Scattered From Dielectric Objects of Uncertain Shapes Using a Multilevel Monte Carlo Scheme

Alexander Litvinenko, İsmail Enes Uysal, Hüseyin Arda Ülkü, Jesper Oppelstrup, Raúl Tempone, and Hakan Bağcı

Simulators capable of computing scattered fields from objects of uncertain shapes are highly useful in electromagnetics and photonics, where device designs are typically subject to fabrication tolerances. Knowledge of statistical variations in scattered fields is useful in ensuring error-free functioning of devices. Oftentimes such simulators use a Monte Carlo (MC) scheme to sample the random domain, where the variables parameterize the uncertainties in the geometry. At each sample, which corresponds to a realization of the geometry, a deterministic electromagnetic solver is executed to compute the scattered fields. However, to obtain accurate statistics of the scattered fields, the number of MC samples has to be large. This significantly increases the total execution time. In this work, to address this challenge, the Multilevel MC (MLMC [1]) scheme is used together with a (deterministic) surface integral equation solver. The MLMC achieves a higher efficiency by “balancing” the statistical errors due to sampling of the random domain and the numerical errors due to discretization of the geometry at each of these samples. Error balancing results in more (less) number of samples requiring coarser (finer) discretizations. Consequently, total execution time is significantly shortened. Numerical results demonstrating the efficiency of this proposed simulator are presented.

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Poster session VI

Reactive Computational Fluid Dynamics

VI-1

Spectral uncertainty analysis of ionic reactions in methane combustion

Daesang Kim, Jie Han, Fabrizio Bisetti, and Omar Knio

The impact of uncertain rate parameters on the evolution of ionic species in methane combustion is analyzed using an adaptive, pseudo-spectral, projection (aPSP) algorithm. A reaction pathway analysis is first conducted to identify key uncertainties. Consequently, attention is focused on the uncertain rates involving all 15 ionic reactions, and 7 elementary reactions involving CH. The uncertainty ranges in the corresponding rate constants are selected first from the UMIST database when available, whereas the remaining uncertainty ranges are selected based on either ADO theories or experimental studies. The aPSP algorithm is used to propagate reaction rate uncertainties in ignition simulations, which enables us to efficiently construct suitable surrogates of the evolution of ionic species concentrations. A global sensitivity analysis is then conducted to identify the dominant source of uncertainty for individual ions. The results indicate that the concentration of free electrons is primarily affected by key neutral reactions affecting the concentration of CH, as well as the chemi-ionization and recombination reactions. The response of the dominant cation, H_3O^+ , exhibits a similar trend, except for an early time dependence on a proton transfer reaction. The computations are also used to investigate the behavior of peak concentrations and of time scales, and to explore their use as observables in methane ignition experiments.

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VI-2

Optimal experimental design of Furan shock tube kinetic experiments

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

A Bayesian optimal experimental design methodology has been developed and applied to refine the rate coefficients of elementary reactions in Furan combustion. Furans are considered as potential renewable fuels. We focus on the Arrhenius rates of $\text{Furan} + \text{OH} \rightleftharpoons \text{Furyl-2} + \text{H}_2\text{O}$, and $\text{Furan} + \text{OH} \rightleftharpoons \text{Furyl-3} + \text{H}_2\text{O}$, and rely on the OH consumption rate as experimental observable. A polynomial chaos surrogate is first constructed using an adaptive pseudo-spectral projection algorithm. The PC surrogate is then exploited in conjunction with a fast estimation of the expected information gain in order to determine the optimal design in the space of initial temperatures and OH concentrations.

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Poster session VII
Other Applications

VII-1

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

Jesper Karlson, Stig Larsson, Mattias Sandberg, Anders Szepessy and 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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VII-2

Kuramoto model for infinite graphs with kernels

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In this paper we study the Kuramoto model of weakly coupled oscillators for the case of non trivial network with large number of nodes. We approximate of such configurations by a McKean-Vlasov stochastic differential equation based on infinite graph. We focus on circulant graphs which have enough symmetries to make the computations easier. We then focus on the asymptotic regime where an integro-partial differential equation is derived. Numerical analysis and convergence proofs of the Fokker-Planck-Kolmogorov equation are conducted. Finally, we provide numerical examples that illustrate the convergence of our method.

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VII-3

On the detectability of transverse cracks in laminated composites using electrical potential change measurements

Lakshmi Selvakumaran, Quan Long, Serge Prudhomme and Gilles Lubineau

Real-time health monitoring of structures made of laminated composites is necessary as significant damage may occur without any visible signs on the surface. Inspection by Electrical Tomography (ET) seems a viable approach that relies on voltage measurements from a network of electrodes across the inspected domain to infer conductivity change within the bulk material. If conductivity decreases significantly with increasing damage, the obtained conductivity map can be correlated to the degradation state of the material. We focus here on detection of transverse cracks. As transverse cracks modify the in-plane transverse conductivity of a single ply, we expect them to be detectable by electrical measurements. Yet, the quality of detection is directly related to the sensitivity of the measurements to the presence of cracks. We use numerical experiments to demonstrate that the sensitivity depends on several material and geometrical parameters. Based on the results, the applicability of ET to detect transverse cracks is discussed. One conclusion from the study is that detecting transverse cracks using ET is more reliable in some laminate configurations than in others. Recommendations about the properties of either the pristine material or the inspected structures are provided to establish if ET is reliable in detecting transverse cracks.

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VII-4

Flow, transport and diffusion in random geometries II: applications

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Multilevel Monte Carlo (MLMC) is an efficient and flexible solution for the propagation of uncertainties in complex models, where an explicit parametrization of the input randomness is not available or too expensive. We present several applications of our MLMC algorithm for flow, transport and diffusion in random heterogeneous materials. The absolute permeability and effective diffusivity (or formation factor) of micro-scale porous media samples are computed and the uncertainty related to the sampling procedures is studied. The algorithm is then extended to the transport problems and multiphase flows for the estimation of dispersion and relative permeability curves. The impact of water drops on random structured surfaces, with microfluidics applications to self-cleaning materials, is also studied and simulated. Finally the estimation of new drag correlation laws for poly-dispersed dilute and dense suspensions is presented.

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Uncertainty Quantification in Porous Media with Multi-Level Monte Carlo

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Geological storage of CO₂ is an attempt at controlling future climate changes. Modelling and simulation of underground CO₂ storage are however subjected to significant sources of geological uncertainties, which requires the use of stochastic approaches. Sources of uncertainties in the CO₂ storage problem can be classified as either geological, physical, or operational uncertainties. Ranking the importance of the model parameters based on their influence can provide a better understanding of the system. Computationally efficient methods for sensitivity analysis, uncertainty quantification, and probability risk assessment are therefore needed. Furthermore, due to the computational complexity of such problems, as even a single deterministic simulation may require parallel high-performance computing, stochastic simulation techniques based on standard Monte Carlo are currently inefficient for these problems. To overcome the prohibitive computational cost of standard Monte Carlo, we propose a Multi-Level Monte Carlo technique to estimate statistical quantities of interest within some prescribed accuracy constraint. We illustrate and verify our proposed approach by a comparison with a Monte Carlo simulation using a common benchmark problem for CO₂ injection. We obtain a significant computational speed-up compared with Monte Carlo.

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VII-6

2-stage adaptive robust optimization of the self-scheduling and market involvement for an electricity producer

Ricardo Lima, Augusto Q. Novais, Antonio J. Conejo

This work address the optimization under uncertainty of the self-scheduling, forward contracting, and pool involvement of an electricity producer operating a mixed power generation station, which combines thermal, hydro and wind sources, and uses a two-stage adaptive robust optimization approach. In this problem the wind power production and the electricity pool price are considered to be uncertain, and are described by uncertainty convex sets. Two variants of a constraint generation algorithm are proposed, namely a primal and dual version, and they are used to solve two case studies based on two different producers. Their market strategies are investigated for three different scenarios, corresponding to as many instances of electricity price forecasts. The effect of the producers' approach, whether conservative or more risk prone, is also investigated by solving each instance for multiple values of the so-called budget parameter. It was possible to conclude that this parameter influences markedly the producers' strategy, in terms of scheduling, profit, forward contracting, and pool involvement. Regarding the computational results, these show that for some instances, the two variants of the algorithms have a similar performance, while for a particular subset of them one variant has a clear superiority.

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VII-7

Multilevel adaptive reaction-splitting simulation method for stochastic reaction networks

Alvaro Moraes, Raúl Tempone and Pedro Vilanova

This work is a generalization of our Multilevel Chernoff Tau-leap method that allow us to accurately estimate averages of observables of Stochastic Reaction Networks. Here, we adaptively split the set of reactions into two categories: fast and slow. Fast reactions are simulated by the Chernoff tau-leap method, while the slow ones are simulated using the modified next reaction method by D. Anderson. This approach defines a mixed method of approximate path simulation. By introducing a hierarchy of time discretization levels, we first show how to couple two mixed paths. Then, we define a Multilevel Monte Carlo estimator for the expected value of any observable based on the state of the process at a fixed final time T .

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Multiscale Modeling of Wear Degradation

Alvaro Moraes, Fabrizio Ruggeri, Raúl Tempone and Pedro Vilanova

Cylinder liners of diesel engines used for marine propulsion are naturally subjected to a wear process, and may fail when their wear exceeds a specified limit. Since failures often represent high economical costs, it is utterly important to predict and avoid them.

In this work, we model the wear process using a pure jump process. Therefore, the inference goal here is to estimate: the number of possible jumps, its sizes, the coefficients and the shapes of the jump intensities.

We propose a multiscale approach for the inference problem that can be seen as an indirect inference scheme.

We found that using a Gaussian approximation based on moment expansions, it is possible to accurately estimate the jump intensities and the jump amplitudes. We obtained results equivalent to the state of the art but using a simpler and less expensive approach.

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VII-9

A Variational Multi-Scale method with spectral approximation of the sub-scales.

Ben Mansour Dia and Tomas Chácon Rebollo

We introduce a variational multi-scale method where the sub-grid scales are computed by spectral approximations. It is based upon an extension of the theorem to non necessarily self-adjoint elliptic operators that have an associated base of eigenfunctions which are orthonormal in weighted L^2 spaces. This allows to element-wise calculate the sub-grid scales by means of the associated spectral expansion. We propose a feasible VMS-spectral method by truncation of this spectral expansion to a finite number of modes. We apply this general framework to the convection-diffusion equation, by analytically computing the family of eigenfunctions. We perform a convergence and error analysis. We also present some numerical tests that show the stability of the method for an odd number of spectral modes, and an improvement of accuracy in the large resolved scales, due to the adding of the sub-grid spectral scales.

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VII-10

Cooperative game for fish harvesting and pollution control.

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We study fishery strategies in a shallow river subject to agricultural and industrial pollution. The flowing pollutants in the river are modeled by a nonlinear stochastic differential equation in a general manner. The logistic growth model for the fish population is modified to cover the pollution impact on the fish growth rate. A stochastic cooperative game is formulated to design strategies for preserving the fish population by controlling the pollution as well as the harvesting fish.

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Optimizing coarse grained models for non equilibrium molecular systems: Dynamical force matching across scales

Vagelis Harmandaris, Evangelia Kalligiannaki, Markos A. Katsoulakis and Petr Plecháč

We study information theoretic quantities as a tool for optimizing proposed parametrized reduced models for non equilibrium systems. Specifically we consider the relative entropy on path space between a given atomistic and a proposed reduced model as a measure for the information loss introduced with coarse graining. We represent the atomistic and reduced models with diffusion processes where the reduced model drift (force) term is parametrized.

In many applications the coarse-grained models are defined by effective potentials or effective dynamics which are sought in a family of parameter-dependent functions, i.e. force, potential. Force matching, inverse Boltzmann, inverse Monte Carlo, relative entropy minimization methods provide optimal parametrization of coarse grained models by minimizing a fitting functional at equilibrium. At non-equilibrium we cannot work with equilibrium distributions since the primary information about the non-equilibrium system is represented by the dynamics. Moreover, the non-equilibrium steady state (NESS) is often not known explicitly.

In this work we propose minimizing the relative entropy (RE) of the path space measures over the parameter space, parametrizing the coarse grained dynamics drift. We prove that the RE minimization problem reduces to a simplified and computationally tractable form, that is further simplified when considering systems in the stationary regime. For stationary systems the fitting functional is the Relative Entropy Rate (RER). We prove that the RER minimization is equivalent to a force matching type problem that has information for the system dynamics. The method directly extends recent relative entropy and force-matching equilibrium methodologies, to non-equilibrium dynamics. Applications of our results are studied for the Langevin dynamics and overdamped Langevin dynamics demonstrating the applicability of the proposed method to singular and non-singular diffusions. A direct study of the RER minimization for the discretized Langevin and overdamped Langevin dynamics is verifying the validity of the continuous time optimal coarse grained model for the corresponding time discretized schemes.

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