WORKSHOP REPORT
On Uncertainty Quantification in Computational Science and Engineering

1. EXECUTIVE SUMMARY:

A successful workshop on Uncertainty Quantification was held on April 26-30, 2013 at King Abdullah University of Science & Technology in Thuwal, KSA. The following report summarizes the observations, recommendations and feedback from the workshop. The workshop featured tutorials on April 26 and 27, public lectures, demonstrations and poster sessions on April 28, 29, and 30. The workshop covered new advances in methods and algorithms for uncertainty quantification, verification & validation (VV), strategic decision-making and applications in green wireless communications, large scale electromagnetics, and clean combustion, among others. The workshop had 37 external and internal participants from academia and industry.

The workshop offered over 11 presentations from renowned experts highlighting the latest research, innovations and business policies surrounding the entire range of uncertainty quantification, green communications, clean combustion, computational fluid dynamics, and large-scale electromagnetics.

2. ADVISORY BOARD MEMBERS:

1: LAST NAME: El-Bakry	First Name: Amr	Title: Dr.	Institution: Exxon-Mobil
2: LAST NAME: Hesthaven	First Name: Jan	Title: Prof	Institution: Brown University
3: LAST NAME: Kaveh	First Name: Mostafa	Title: Prof.	Institution: University of Minnesota
4: LAST NAME: Klie	First Name: Hector	Title: Dr.	Institution: Conocophillips
5: LAST NAME: Majda	First Name: Andrew	Title: Prof.	Institution: New York University
6: LAST NAME: Matthies	First Name: Hermann	Title: Prof.	Institution: TU, Germany
7: LAST NAME: Michielssen	First Name: Eric	Title: Prof.	Institution: University of Michigan
8: LAST NAME: Najm	First Name: Habib	Title: Dr.	Institution: Sandia National Lab.

3. WORKSHOP ORGANISERS:

Raul Tempone, SRI UQ Center Director, King Abdullah University of Science and Technology.

Omar Knio, SRI UQ Center Deputy Director, King Abdullah University of Science and Technology.

4. WORKSHOP DESCRIPTION:

The main purpose of the workshop was to:

(i) give tutorials, helping young researchers to insert themselves in the latest UQ-VV results;
(ii) survey advances by SRI-UQ members and leading experts;
(iii) Disseminate latest results of UQ to academic and industrial experts from inside and outside of the Kingdom;
(iv) Review meeting on the research directions of the UQ Center.

5. LISTS OF SPEAKERS:

1: LAST NAME: Alouini	First Name: Slim	Title: Prof.	Institution: KAUST
2: LAST NAME: Bagci	First Name: Hakan	Title: Ass. Prof.	Institution: KAUST
3: LAST NAME: Bisetti	First Name: Fabrizio	Title: Ass. Prof.	Institution: KAUST
4: LAST NAME: Le Maitre	First Name: Olivier	Title: Prof.	Institution: CNRS
5: LAST NAME: Nobile	First Name: Fabio	Title: Prof.	Institution: EPFL
6: LAST NAME: Prudhomme	First Name: Serge	Title: Prof.	Institution: Ecole Polytechnique Montreal
7: LAST NAME: Rezki	First Name: Zouheir	Title: Dr.	Institution: KAUST
8: LAST NAME: Ruggeri	First Name: Fabrizio	Title: Prof.	Institution: CNR-IMATI, ITALY
9: LAST NAME: Scavino	First Name: Marco	Title: Prof.	Institution: URM, Uruguay
10: LAST NAME: Tembine	First Name: Hamidou	Title: Dr.	Institution: KAUST
11: LAST NAME: Tempone	First Name: Raul	Title: Associate Prof.	Institution: KAUST

SRI Center for Uncertainty Quantification Annual Meeting.
April 26-30, 2013

	Fri April 26	Sat April 27	Sun April 28	Mon April 29	Tue April 30
9:00 – 9:30	Tutorial Ia: UQ intro tutorial RAUL TEMPONE / FABIO NOBILE	Tutorial IV: Communication at Low Power Regime: Energy Efficiency and Effect of Uncertainty. SLIM ALOUINI / ZOUHEIR REZKI	**Center presentation for Board Members** (reserved to at KAUST and external participants of SRI UQ).		Local Meetings
9:30 – 10:00				Lecture 3: On the Estimation of the Expected Information Gain for Bayesian Experimental Designs MARCO SCAVINO	
10:00 – 10:30				Lecture 4: An Accurate and Efficient Discontinuous Galerkin Finite Element Method for Solving Time Domain Maxwell Equations HAKAN BAGCI	
10:30 – 11:00	Break	Break	Break	Break	
11:00 – 11:30	Tuturial Ib: UQ intro tutorial RAUL TEMPONE / FABIO NOBILE	Tutorial IIIb: An introduction to bayesian statistics through some case studies FABRIZIO RUGGERI	Lecture 1: Galerkin Method for Stochastic Ordinary Differential Equations with Uncertain Parameters OLIVIER LE MAITRE	Lecture 5: Quantification of uncertainty in ion chemistry parameters for combustion applications FABRIZIO BISETTI	
11:30 – 12:00			Lecture 2: Overview of the research activities at the communication theory lab at Kaust SLIM ALOUINI	Lecture 6: Verification and Validation SERGE PRUDHOMME	
12:00 – 13:30	Lunch	Lunch	Lunch	Lunch	Lunch
13:30 – 14:00	Tutorial IIa: Nonasymptotic Mean Field Games	Tutorial Iib: Nonasymptotic Mean Field Games	**Advisory Board Meeting**	**Advisory Board Meeting**	Local Activities
14:00 – 14:30	HAMIDOU TEMBINE	HAMIDOU TEMBINE			
14:30 – 15:00	Break	Break			
15:00 – 15:30	Tutorial IIIa: An introduction to bayesian statistics through some case studies FABRIZIO RUGGERI	Poster set-up	**Board Members Discussion**	Discussion time.	
15:30 – 16:00			Poster Session		
16:00 – 16:30		Welcome Reception in Poster Area			
16:30 – 17:00					
			Conference Dinner: Al- MARSA	Thuwal Dinner: FISH Restaurant	

6. AGENDA:


Speakers: Dr. Raul Tempone & Dr. Fabio Nobile
Date: Friday, April 26
Time: 9:00 to 10:30 am & 11:00 am to 12:00 pm

Title: A brief introduction to probabilistic Uncertainty Quantification

Abstract: We motivate the purpose of uncertainty quantification methodology in practical problems and review standard techniques, like: i) classical sampling methods including Monte Carlo and the recent Multilevel Monte Carlo ii) Generalized Polynomial Chaos and response function methods, like Stochastic Galerkin, Stochastic Collocation and the Random Discrete L2 projection.

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Speaker: Dr. Hamidou Tembine
Date: Friday, April 26 & Saturday, April 27
Time: 1:30 to 2:30 pm

Title: Nonasymptotic Mean Field Games

Abstract: Mean field games have been studied under the assumption of very large number of players. For such large systems, the basic idea consists to approximate "large games" by a stylized game model with a continuum of players. The approach has been shown to be useful in many stylized models in economics and engineering. However, the stylized game model with continuum of decision-makers assumption is rarely observed in practice and the approximation proposed in the asymptotic regime is meaningless for networks with few entities. In this work, we propose a mean-field framework that is suitable not only for large systems but also for a small world with few numbers of entities. The applicability of the proposed framework is illustrated through various examples including queueing mean field game with heterogeneous servers, minority games with asymmetric information and dynamic auction with asymmetric valuation distributions.

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Speaker: Dr. Fabrizio Ruggeri, CNR IMATI - Milano (Italy)
Date: Friday, April 26 & Saturday, April 27
Time: 3:00 to 5:00 pm & 11:00 am to 12:00 pm

Title: An introduction to bayesian statistics through some case studies

Abstract: After a short introduction to ideas and methods typical of the Bayesian approach, they will be shown in practice through the following case studies:
- Bayesian methods in project management
- Hierarchical random effects models for survival in patients with Acute Myocardial Infarction
- Integrating clinicians' opinion in the Bayesian meta-analysis of observational studies: the case of risk factors for falls in community-dwelling older people
- On the use of Bayesian Belief Networks in modelling human and organisational causes of maritime accidents
- Reliability: Gas escapes; Failures of train's door; Software reliability
- Predator-prey systems

The tutorial will not enter in too many technical details but the case studies will give the opportunity to show how to perform a Bayesian analysis and some of its benefits and critical aspects.

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Speaker: Dr. Slim-Alouini & Dr. Zouheir Rezki
Date: Saturday, April 27
Time: 9:00 to 10:30 am

Title: Communication at Low Power Regime: Energy Efficiency and Effect of Uncertainty.

Abstract: In many settings, communication should operate at low power regime, or equivalently at low signal-to-noise ratio (SNR). Such is the case, for instance, of wideband communications, cellular networks in some specific (but frequent) cases, sensor networks, etc. This has driven the interest of deriving performance limits of communication at low power regime during the last two decades. Perhaps surprising, communication at low power regime provides generally the best energy efficiency. However, it is not clear how meaningful communication at low power regime is, especially in regard to the limited processing capabilities of mobile devices.

In this talk, we define communication at low power regime, we argue that the low-SNR framework encompasses scenarios where the bandwidth and the power are fixed, but the system degree of freedom is large enough such that the power per degree of freedom is very low. Then, we give an overview of existing results on communication at low power regime. Particularly, we highlight the effect of fading and channel uncertainty at transmit and receive sides. Then, we introduce new recent results characterizing performance limits of communication at low power regime and provide practical schemes that achieve those limits at

asymptotically low power regime. The later characterization includes several typical wireless channel models such as point-to-point communication, multiuser communication and communication under secrecy constraint. As a byproduct of our analysis, a refined characterization of energy efficiency in these cases is also presented.

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Lecture 1:
Speaker: Dr. Olivier Le Maitre, Duke University, Durham, North Carolina, USA
Date: Sunday, April 28
Time: 11:00 to 11:30 am

Title: Galerkin Method for Stochastic Ordinary Di_erential Equations with Uncertain Parameters

Abstract: We propose a Galerkin method for the resolution of a certain class of Stochastic Ordinary Di_erential Equations (SODE) driven by Wiener processes and in-volving some random parameters. The dependence of the solution with respect to the uncertain parameters is treated by Polynomial Chaos expansions, with expansion coe_cients being random processes function of the Wiener processes.
An hybrid Monte-Carlo Galerkin method is then proposed to compute these ex-pansion coe_cients, allowing for a complete uncertainty analysis of the solution. In particular, we show that one can retrieve the dependence on the uncertain parameters of the stochastic noise in the solution. Exemples of applications are shown for linear and non linear SODEs. Finally, the extension of the method to non-intrusive techniques and more general source of stochasticity is discussed. This is a joint work with Omar Knio.

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Lecture 2:
Speaker: Dr. Slim-Alouini, KAUST
Date: Sunday, April 28
Time: 11:30 am to 12:00 pm

Title: Overview of the research activities at the communication theory lab at Kaust

Abstract: The concept of cognitive networks has recently emerged as one of the efficient means for utilizing the scarce spectrum by allowing spectrum sharing between a licensed primary network and a secondary network. In this talk, we briefly present an overview of various recently proposed types of cognitive networks and then discuss some fundamental capacity results of these networks. The talk goes then over the potential offered by free space optical communications to relieve spectrum scarcity and then summarizes the main challenges that need to be surpassed before such kind of systems can be deployed.

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Lecture 3:

Speaker: Dr. Marco Scavino, Universidad de la Republica, Montevideo, Uruguay
Date: Monday, April 29
Time: 09:30 to 10:00 am

Title: On the Estimation of the Expected Information Gain for Bayesian Experimental Designs

Abstract: The Shannon-type expected information gain is a relevant measure to rank computer designed experiments before the real data are available. For realistic physical models, especially for those involving the solution of partial differential equations, fast computational methods are needed to estimate such gain.

We propose to use the Laplace approximation for the integration of the posterior probability density function, in order to accelerate the estimation of the expected information gains in the model parameters and in the predictive quantities of interest. Asymptotic forms for the Shannon mutual informations are also obtained in the case of models with unidentifiable parameters.

Some examples with nonlinear models, among them the design of the boundary source locations for impedance tomography in a square domain, illustrate the performance of the proposed method of estimation.

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Lecture 4:

Speaker: Dr. Hakan Bagci, KAUST
Date: Monday, April 29
Time: 10:00 to 10:30 am

Title: An Accurate and Efficient Discontinuous Galerkin Finite Element Method for Solving Time Domain Maxwell Equations

Abstract: Increasing complexity of modern electronic systems renders error control in simulation-based design frameworks more challenging. Electromagnetic simulation tools, which are indispensible components of such frameworks, must be capable of employing higher-order space and time discretization schemes to provide accurate results efficiently even when they are used for analyzing wave interactions on highly complex systems.

To this end, discontinuous Galerkin finite element methods (DG-FEM) are becoming an alternative to finite difference time-domain methods for analyzing transient electromagnetic wave interactions. The DG-FEM formulation weakly enforces the continuity of the fields and uses numerical flux to realize information exchange across boundaries of spatial discretization elements. Use of numerical flux results in localized spatial operations and equips DG-FEM with several computationally desired properties.

In this talk, we will describe a DG-FEM solver that makes use of a recently developed time integration scheme and exact absorbing boundary conditions to achieve highly improved

efficiency and accuracy. The new time integration scheme assumes the traditional $PE(CE)^m$ form; however predictor-corrector coefficients are obtained using a numerical scheme with fully controllable accuracy. This approach allows the accuracy of time integration to be set as desired to match the accuracy of the higher-order spatial discretization. The use of exact absorbing boundary conditions, which are analytically derived from the radiation conditions of the outgoing wave modes, and their higher-order discretization allow for the accuracy of the computation domain truncation to match that of the DG-FEM for all orders of spatial basis functions. For increased efficiency, the computation of the discretized temporal convolutions pertinent to the boundary conditions is accelerated using a blocked FFT scheme without introducing additional numerical errors.

Numerical examples will demonstrate that the proposed DG-FEM uses much larger time steps than the DG-FEM with a classical time integration schemes. Additionally, it will be shown that it can achieve ten/eleven digits of accuracy when higher-order spatial basis functions are used to discretize the Maxwell equations as well as the absorbing boundary conditions.

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Lecture 5:
Speaker: Dr. Fabrizio Bisetti, KAUST
Date: Monday, April 29
Time: 11:00 to 11:30 am

Co-authors: F. Rizzi, K. W. Cheng, J. Han, and O. Knio

Title: Quantification of uncertainty in ion chemistry parameters for combustion applications

Abstract: Ion and electron chemistry in reactive flows has received significant attention in recent years due to its potential for efficiency enhancement and emission reduction in combustion systems. In this talk I will present recent work on the characterization of the impact of uncertainty in reaction rate parameters on the temporal evolution of electron and ion number densities in shock tubes. A thorough description of the mathematical framework at the basis of shock tube simulations is presented alongside the main results on the sensitivities of model predictions to key reactions.

Lecture 6:
Speaker: Dr. Serge Prudhomme, Ecole Polytechnique de Montreal, Montreal, Canada
Date: Monday, April 29
Time: 11:30 to 12:00 pm

Title: Verification and Validation

Abstract: The purpose of this presentation is to briefly review concepts of verification and validation and describe some research work on the subject conducted at the center. In particular, we will present preliminary work on a posteriori error estimation for solution verification of approximations of stochastic partial differential equations. The error estimates can be used to adaptively refine both the physical and stochastic discretizations. The approach relies on the ability to decompose the error into contributions from the physical discretization error and from the response surface approximation error in stochastic, or parameter, space. Our decomposition of the errors and adaptive technique allows one to optimally use available resources to accurately estimate and quantify the uncertainty in a specific quantity of interest (QoI).

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7. POSTERS:

Poster 1.

Authors: P. Ubaidulla, Mohamed-Slim Alouini, and Sonia Aïssa

Title: Cognitive Relay Precoder Designs and Power Allocation under Channel State Uncertainties.

Abstract: We present robust joint relay precoder designs and transceiver power allocations for a cognitive radio network under imperfect channel state information (CSI). The secondary (or cognitive) network consists of multiple pairs of single-antenna transceiver nodes and non-regenerative two-way relays with multiple antennas that aid the communication process between the transceiver pairs. The secondary nodes share the spectrum with a licensed primary user (PU) while guaranteeing that the interference to the PU receiver is maintained below a specified threshold. The proposed precoder designs ensure robust performance in the presence of errors in the channel state information (CSI). Such robust designs are of significant interest since in practice it is very difficult to obtain perfect CSI.
We consider CSI uncertainties with two different types of characterization and corresponding robust designs. First, we consider robust relay precoder designs and power allocation that are applicable when CSI errors have known first and second moments. In this case, we propose stochastically robust designs. Next, we consider precoder designs and power allocation that are applicable when the CSI error can be characterized in terms of a spherical uncertainty region. In this case, we propose worst-case robust designs. We show that the proposed designs can be reformulated as convex optimization problems that can be solved efficiently even though the original problems are mathematically intractable. We illustrate the performance of the proposed designs through some selected numerical simulations.

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Poster 2.

Authors: Lokman Sboui, Zouheir Rezki, Mohamed-Slim Alouini

Title: Low SNR Cognitive Radio Capacity

Abstract: We study the ergodic capacity of Cognitive Radio (CR) spectrum sharing systems at low power regime for Nakagami fading channels. We formally define the low power regime and present closed form expressions of the capacity at low power regime under various types of interference and/or power constraints, depending on the available channel state information (CSI) of the cross link (CL) between the secondary user transmitter and the primary user receiver. We explicitly characterize two regimes where either the interference constraint or the power constraint dictates the optimal power profile. Our framework also highlights the effects of different fading parameters on the secondary link ergodic capacity.
We, also, study more realistic scenarios when there is either a 1-bit quantized channel feedback from the CL alone or from both the CL and the secondary link (SL), and propose simple power control schemes and show that these schemes are capacity-achieving at asymptotically low power regime.
Interestingly, we show that the low power regime analysis provides a specific insight on the capacity behavior of CR that has not been reported by previous studies.

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Poster 3.

Authors: Hakim Ghazzai, Mohamed-Slim Alouini

Title: Smart Grid Energy Procurement for Green LTE Cellular Networks.

Abstract: In this study, we implement a green heuristic algorithm involving the Base Station (BS) sleeping strategy that aims to ensure energy saving for the radio access network of the 4G-LTE (Fourth Generation Long Term Evolution) mobile networks. We propose an energy procurement model that takes into consideration the existence of multiple energy providers in the smart grid power system (e.g. fossil fuel and renewable energy sources, etc.) in addition to deployed photovoltaic (PV) panels in BS sites. Moreover, the analysis is based on the dynamic time variation of daily traffic and aims to maintain the network Quality of Service (QoS). Our simulation results show an important contribution in the reduction of CO2 emissions that can be reached by optimal power allocation over the active BSs.

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Poster 4.

Authors: Muhammad Mehboob Fareed and Mohamed-Slim Alouini

Title: Efficient Incremental Relaying

Abstract: We propose a novel relaying scheme which improves the spectral efficiency of cooperative diversity systems by utilizing limited feedback from destination. Our scheme capitalizes on the fact that relaying is only required when direct transmission suffers deep fading. We calculate the packet error rate for the proposed efficient incremental relaying scheme with both amplify and forward and decode and forward relaying. Numerical results are also presented to verify their analytical counterparts.

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Poster 5.

Authors: Hamza Soury, Ferkan Yilmaz, Mohamed-Slim Alouini.

Title: Symbol Error Probability of M-QAM over Generalized Fading Channels subject to Generalized Gaussian Noise.

Abstract: This work considers the average symbol error probability of square Quadrature Amplitude Modulation (QAM) coherent signaling over flat fading channels subject to additive generalized Gaussian noise. More specifically, a generic closed-form expression in terms of the Fox H function and the bivariate Fox H function is offered for the extended generalized-K fading case. Simplifications for some special fading distributions such as generalized-K fading, Nakagami-m fading, and Rayleigh fading and special additive noise distributions such as Gaussian and Laplacian noise are then presented.

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Poster 6.

Authors: Jian Qi, Sonia Aissa, and Mohamed-Slim Alouini

Title: Impact of I/Q Imbalance on the Performance of Two-Way CSI-Assisted AF Relaying

Abstract: In this paper, we investigate half-duplex two-way dual-hop channel state information (CSI)-assisted amplify-and-forward (AF) relaying in the presence of in-phase and quadrature-phase (I/Q) imbalance. A compensation approach for the I/Q imbalance is proposed, which employs the received signals together with their conjugations to detect the desired signal. We also derive the average symbol error probability of the considered half-duplex two-way dual-hop CSI-assisted AF relaying networks with and without compensation for I/Q imbalance in Rayleigh fading channels. Numerical results are provided and show that the proposed compensation method mitigates the impact of I/Q imbalance to a certain extent.

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Poster 7.

Author: Fatma Benkhelifa, Zouheir Rezki, Mohamed-Slim Alouini

Title: Low SNR Capacity of FSO Links over Gamma-Gamma Atmospheric Turbulence Channels.

Abstract: In this paper, we study the ergodic capacity of free space optical communication systems over Gamma-Gamma atmospheric turbulence fading channels with perfect channel state information at both the transmitter and the receiver. In our framework, we mainly focus on the low signal-to noise ratio range and show that the ergodic capacity scales proportionally to SNR log^4(1/SNR). We show also that one-bit CSI feedback at the transmitter is enough to achieve this capacity using an on-o ff power control scheme.

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Poster 8.

Authors: Hamidou Tembine, Raul Tempone, Pedro Vilanova

Title: Distributed Strategic Learning

Abstract: This work presents some of the essential ingredients of learning in games, particularly coalitional learning, reinforcement learning, cost-of-learning, Q-learning, mean-field learning, combined learning, heterogeneous learning, hybrid learning and speedup learning.
We emphasize a stochastic approximation approach (probabilistic and dynamical system perspectives) and present one of the major challenges in the design of large-scale systems: the need for fully distributed learning algorithm schemes that consume a minimal amount of resources with a minimal amount of information exchange and yet with a very fast convergence time.

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Poster 9.

Authors: Hamidou Tembine, Raul Tempone, Pedro Vilanova

Title: Mean Field Stochastic Games

Abstract: This note introduces recent advances in mean field stochastic games in large-scale systems. The main results are related to the following configurations (i) discrete time microscopic Markovian interaction to macroscopic object, (ii) Macroscopic stochastic evolution, (iii) from microscopic evolution in continuous time to its mean field limit and, (iv) risk-sensitive mean field games in large populations, (iv) non-asymptotic mean field games.

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Poster 10.

Authors: Abdul-Lateef Haji-Ali Raul Tempone

Title: Mean-field Limit of Pedestrian Model

Abstract: We study the mean-field limit of a particle-based system modeling the behavior of many indistinguishable pedestrians as their number increases. The base model is a modified version of Helbing's social force model [1]. In the mean-field limit, the time-dependent density of two-dimensional pedestrians satisfies a four-dimensional integro-differential Fokker-Planck equation [2]. To approximate the solution of the Fokker-Planck equation we use a time-splitting approach and solve the diffusion part using a Crank-Nicholson method. The advection part is solved using a Lax-Wendroff-Leveque method or an upwind Backward Euler method depending on the advection speed. Moreover, we use multilevel Monte Carlo to estimate observables from the particle-based system. We discuss these numerical methods, and present numerical results showing the convergence of observables that were calculated using the particle-based model as the number of pedestrians increases to those calculated using the probability density function satisfying the Fokker-Planck equation.
We look at two cases. Case 1 is a one-dimensional test case in which pedestrians move clockwise on a circle with no obstacles. One the other hand, Case 2 is a more realistic two dimensional case in which pedestrians move towards an exit in an environment with static obstacles.

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Poster 11.

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

Title: Adaptive Multilevel Monte Carlo With Simultaneous Weak and Strong Error Control

Abstract: We consider the Multilevel Monte Carlo (MLMC) method in applications involving differential equations with random data where the underlying approximation method of individual samples is based on uniform spatial discretizations of arbitrary approximation order and cost. We perform a general optimization of the parameters defining the MLMC hierarchy in such cases.
The resulting hierarchies are different from typical MLMC hierarchies; in particular they do not have a fixed ratio between successive mesh sizes. Moreover, our optimization yields a nontrivial splitting of tolerance between bias and statistical errors that is usually different from the value 1=2, traditionally used in MLMC.
We present numerical results, applying our method to an elliptic PDE with stochastic coefficients. We emphasize how the optimal hierarchies change from the standard MLMC method depending on problem parameters, such as the solver cost function.

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Poster 12.

Authors: Mohammad Motamed, Fabio Nobile and Raul Tempone

Title: Stochastic Wave Equation: Analysis and Computation

Abstract: We propose a stochastic collocation method for solving the second order acoustic wave equation in a heterogeneous random medium with a piece- wise smooth random wave speed and subjected to deterministic boundary and initial conditions. The medium consists of non-overlapping sub- domains. In each sub-domain, the wave speed is smooth and is given in terms of one random variable. We assume that the interfaces of speed discontinuity are smooth. One important example is wave propagation in multi-layered media with smooth interfaces. The numerical scheme consists of a finite difference or finite element method in the physical space and a collocation in the zeros of suitable tensor product orthogonal polynomials (Gauss points) in the probability space. We provide a rigorous convergence analysis and demonstrate different types of convergence of the probability error with respect to the number of collocation points under some regularity assumptions on the data. In particular, we show that, unlike in elliptic and parabolic problems, the solution to hyperbolic problems is not in general analytic with respect to the random variables. Therefore, the rate of convergence is only algebraic. A fast spectral rate of convergence is still possible for some quantities of interest and for the wave solution with particular types of data. We show that analytical results and numerical examples are consistent and that the stochastic collocation method may be a valid alternative to the more traditional Monte Carlo method.

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Poster 13

Authors: Regis Cottereau

Title: A coupling method for stochastic problems. Application to random homogenization

Abstract: The poster describes a multiscale strategy that allows to couple stochastic and deterministic models as well as two stochastic models described at different scales. The transition condition enforced between the two models is weak, in the sense that it is based on volume coupling in space (rather than more classical boundary coupling) and on a volume/sample average in the random dimension. The poster then presents an application of this weak coupling technique for the development of a new iterative method for the homogenization of random media. The technique is based on the coupling of the stochastic microstructure to a tentative homogenized medium, the parameters of which are initially chosen at will. Based on the results of the coupled simulation, for which Dirichlet or Neumann boundary conditions are posed at the boundary of the tentative homogenized medium, the parameters of the homogenized medium are then iteratively updated. An example shows the efficiency of the proposed approach compared to the classical KUBC and SUBC approaches in stochastic homogenization.

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Poster 14

Authors: Matteo Icardi, Daniele Marchisio, Serge Prudhomme; Rajandrea Sethi, Raul Tempone; Tiziana Tosco

Title: Multi-scale simulation and Bayesian inversion of advection-diffusion-reaction equation in porous media.

Abstract: The mathematical models for particle and contaminant transport in subsurface flows are often limited by a lack of knowledge on the equation parameters. In this work pore-scale three-dimensional simulations of solute transport in a complex porous structure are analyzed to obtain macro-scale averaged quantities. These quantities can be used to select the appropriate model equations for macro-scale transport and estimate the parameters of the resulting advection-dispersion-reaction macro-scale equations. The parameters considered are the effective velocity, effective porosity, dispersion and transfer coefficient. Bayesian inversion techniques are used to solve the inverse problem with a collocation approach or with Markov Chain Monte-Carlo. The macro-scale forward model is solved either by a simplified analytical formulation or by standard finite difference method while the pore-scale data are obtained from expensive Computational Fluid Dynamics finite volume simulations. Correlation laws that links the inner scale flow properties and porous structures with the macro-scale parameters are proposed.

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Poster 15

Author: Bilal Saad

Title: Study of a numerical scheme for two-phase two-component flow in porous media and application to nuclear waste storage.

Abstract: An important quantity of hydrogen can be produced by corrosion of the steel engineered barriers (carbon steel overpack and stainless steel envelope) of radioactive waste packages. There is growing awareness of this production that the effect of hydrogen gas generation can affect all the functions allocated to the canisters, waste forms, backfill, host rock. Host rock safety function may be threaten by over pressurization leading to opening fractures of the domain, inducing groundwater flow and transport of radionuclides.
In nuclear waste management, the migration of gas through the near field environment and the host rock, involves two components, water and pure hydrogen; and two phases liquid and gas. We do not only have two different phases (liquid and gas) but also two components (water and hydrogen) in each phase. Then, the mathematical model, describing the gas migration in porous media, consists to write the mass conservation of the component water in the liquid phase (no vapor of water due to evaporation) and of the component hydrogen in both phases since the hydrogen is present in a dissolved and gasous form. The solubility of the components in the phases is taken into account by considering the Henry law. This problem renews the mathematical and numerical interest in the equation describing multiphase multicomponent flows through porous media.
In this work, we address the construction and convergence analysis of a finite volume scheme, based on a two pressures formulation, for two–component two–compressible flow without simplified assumptions on the state law of the density of each phase and including gravity and capillary effects, with a special regard to radioactive waste storage in geologic formations. This scheme consists in a finite volume method together with a phase-by-phase upstream scheme. The implicit finite volume scheme satisfies industrial constraints of robustness and stability.
Finally we also address one of the outstanding physical and mathematical problems in multiphase flow simulation: the appearance disappearance of one of the phases, leading to the degeneracy of the equations satisfied by the saturation. The Couplex-Gas benchmark was proposed by the ANDRA 1 and the research team MoMas 2 in order to improve the simulation of the migration of hydrogen, generated some interest and engineers encountered difficulties in handling the appearance and disappearance of the phases. We present the ability of our numerical approximation method, based on a two pressures formulation in the case where both phases are miscible, to actually cope with the appearance or/and disappearance of one phase.

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Poster 16:

Authors: Lorenzo Tamellini, Olivier Le Maitre, Anthony Nouy

Title: Proper Generalized Decomposition for Stochastic Navier–Stokes problems

Abstract: We propose an application of the Proper Generalized Decomposition to the stochastic Navier-Stokes equations in the incompressible regime. The method aims at determining the dominant components of the stochastic flow by means of suitable reduced bases approximations. The deterministic reduced basis is here constructed using Arnoldi-type iterations, which involve the resolution of a series of deterministic problems whose structure is similar to the original deterministic Navier-Stokes equations, so that classical solvers can be re-used. The stochastic solution is then approximated in the reduced space of deterministic modes by means of a Galerkin projection, yielding a low dimensional set of coupled quadratic equations for the stochastic coefficients. The efficiency of the method will be illustrated and its computational complexity will be contrasted with the classical Galerkin Polynomial Chaos method. Computation of the reduced solution residual and of the stochastic pressure field will also be presented.

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Poster 17

Authors: Julio Enrique Castrillon Candas, Jun Li, Victor Eijkhout

Title: An Adapted Multi-Level Solver for Large Scale Radial Basis Function Interpolation with applications to Kriging

Abstract: We develop an adapted discrete Hierarchical Basis (HB) to stabilize and efficiently solve the Radial Basis Function (RBF) interpolation problem with finite polynomial order. Applications to the Best Linear Unbiased Estimator regression problem are shown.
The HB forms an orthonormal set that is orthogonal to the space of polynomials of order m defined on the set of nodes $X \subset \mathbb{R}^{3}$. This leads to the decoupling of the RBF problem thus removing the polynomial ill-conditioning dependency from the joint problem. In particular, the adapted HB method works well for higher-order polynomials. We demonstrate results of up to half a million interpolation/observation points. To our knowledge this is the fastest solver for linear and higher polynomial order.

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Poster 18

Authors: Quan Long, Marco Scavino Raul Tempone Suojin Wang

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

Abstract: Shannon-type expected information gain is an important utility in evaluating the usefulness of a proposed experiment that involves uncertainty. Its estimation, however, cannot rely solely on Monte Carlo sampling methods, that are generally too computationally expensive for realistic physical models, especially for those involving the solution of stochastic partial differential equations. In this work we present a new methodology, based on the Laplace approximation of the posterior probability density function, to accelerate the estimation of expected information gain in the model parameters and predictive quantities of interest. Furthermore, in order to deal with the issue of dimensionality in a complex problem, we use sparse quadratures for the integration over the prior. We show the accuracy and efficiency of the proposed method via several nonlinear numerical examples, including a single parameter design of one dimensional cubic polynomial function and the current pattern for impedance tomography.

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Poster 19:

Authors: Ivo Babuska, Zaid Sawlan, Marco Scavino, Barna Szabo, Raul Tempone

Title: Bayesian model comparison for fatigue data

Abstract: Fatigue tests at different speeds (cycles per minute) all along a range of mean loads are used to determine the fatigue strength of a certain specimen. Once that experiments involving expensive destructive tests are carefully designed and applied, a crucial point is how to estimate the reliability fatigue life of the specimen.
To this end, a rigorous statistical framework is needed to support making engineering decision. In this work we present a systematic approach for model calibration, model selection and validation (see Babuška et al., 2008), and prediction of relevant quantities of interest, such as the remaining life of a given specimen.

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Poster 20:

Authors: Alvaro Moraes, Fabrizio Ruggeri, Raul Tempone, Pedro Vilanova

Title: Multiscale Modeling of Wear Degradation in Cylinder Liners

Abstract: 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, and therefore the inference goal is to estimate the coefficients of the jump intensities.
We use a multiscale approach to gradually improve the estimations. This allows to incorporate information obtained using simpler models, i.e. the mean field associated to the pure jump process, in order to ease the estimations.
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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Poster 21:

Authors: Alvaro Moraes, Raul Tempone, Pedro Vilanova

Title: Chernoff-Based Hybrid Tau-Leap

Abstract: 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 SSA and the Chernoff tauleap methods. 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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Poster 22:

Authors: Alvaro Moraes, Raul Tempone, Pedro Vilanova

Title: Multi level Chernoff-Based Hybrid Tau-Leap

Abstract: 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 algorithm for the Chernoff-based hybrid tauleap algorithm. This variance reduction technique 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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Poster 23.

Authors: Christian Bayer, Hakon Hoel, Erik von Schwerin, and Raul Tempone

Title: Non-asymptotic Optimal Stopping Criteria for Monte Carlo

Abstract: Consider the setting of estimating the mean of a random variable by a sequential stopping rule Monte Carlo (MC) method. How do you decide when to stop sampling given the requirement that the error be smaller than a given tolerance, TOL, with a given statistical confidence? An appeal to the Central Limit Theorem leads to the typical second moment based sequential stopping rule MC which generally tends to perform well in the asymptotic regime when TOL ! 0. This poster will show some examples where such a stopping rule is unreliable in the non-asymptotic regime and present a higher moment based stopping rule which is shown in numerical examples to perform more reliably and only slightly less efficiently than the second moment based stopping rule.
The work presented in this poster is a collaboration, and is available as a preprint: C. Beyer, H. Hoel, E. von Schwerin, and R. Tempone, On non-asymptotic optimal stopping criteria in Monte Carlo simulations, MATHICSE technical report 07.2013, mathicse.epfl.ch/page-69806-en.html

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Poster 24.

Authors: Håkon Hoel, Erik von Schwerin, Anders Szepessy, and Raul Tempone.

Title: Implementation and Analysis of an Adaptive Multilevel Monte Carlo Algorithm

Abstract: In 2008 Mike Giles proposed a multilevel Monte Carlo (MLMC) method based on a hierarchy of uniform time meshes for weak approximations of solutions to Ito stochastic differential equations. An impressive feature of this method is the complexity reduction of weak approximations with a mean squared error O(TOL^2) constraint from O(TOL^3) when using a standard single level Monte Carlo method to O(TOL^2 log(TOL)^2) when using the MLMC method. In this poster we present an extension of Giles' MLMC method based on a hierarchy of adaptively refined, on uniform meshes, generated by the adaptive algorithm introduced by Szepessy et al. in the early 2000s. Main theoretical results for our method are presented, showing that the adaptive MLMC method is asymptotically accurate and essentially has the same complexity as Giles' uniform time step MLMC method, but with improved control of asymptotic constants. A numerical example with a barrier problem where we compare the performance of different methods in terms of error vs. cost is also included.

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Poster 25:

Authors: Giovanni Migliorati, Fabio Nobile, E.von Schwerin, Raul Tempone

Title: Analysis of the discrete L2 projection on polynomial spaces with random evaluations

Abstract: This is a joint work with Fabio Nobile (EPFL and Politecnico di Milano), Erik von Schwerin (EPFL and KAUST) and Raul Tempone (KAUST).

In many PDE models the parameters are not known with enough accuracy, or they naturally feature randomness and can be treated therefore as random variables. We consider a smooth parameter-to-solution map (as, for instance, in the Darcy equations for porous media flow, with random permeability [1]) and look for a multivariate polynomial approximation of it (polynomial chaos expansion).

An approach that has been advocated recently ([7, 5, 4]) consists in evaluating the solution on randomly chosen parameters and doing a discrete L2 projection on the polynomial space. This problem can be analyzed in a regression framework [6] with random design. As usual, the regression function minimizes the L2 risk, but here the observations are noise-free evaluations on random points.

Here we restrict our analysis to univariate or multivariate target functions and study the approximation properties of the random L2 projection with respect to the number of sampling points, the maximum polynomial degree, and the smoothness of the function to approximate.

In [2] we prove optimality estimates (up to a logarithmic factor) when the random points are sampled from bounded random variables with strictly positive probability density functions. Our analysis of the random projection proves that the optimal convergence rate is achieved when the number of sampling points scales as the square of the dimension of the polynomial space. Moreover, it gives an insight on the role of smoothness and the conditioning of the random projection operator in the accuracy and stability of the L2 regression.

Several numerical tests [2, 3] confirm our theoretical results, and point out some significant differences between the one-dimensional and the multidimensional cases.

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Poster 26.

Authors: K. W. Cheng, F. Rizzi, J. Han, F. Bisetti, O. M. Knio

Title: Application of Sparse Adaptive Pseudospectral Uncertainty Quantification Scheme to Chemical Ionization in Combustion Systems

Abstract: This study employs an adaptive non-intrusive spectral projection (NISP) approach [1,2] to propagate parametric uncertainties in a proposed kinetic model for chemical ionization in methane combustion involving charged ions. The kinetic model comprises 11 charged species and 67 elementary reactions assembled from existing literature [3]. We investigate the impact of the inherent uncertainties in the reaction rate parameters on the peak concentrations of electrons and selected ions (i.e. H3O+, C2H3O+, HCO+, E-, OH-, O-, CHO2-). These charged species are chosen as quantities of interest (QoIs) due to their role in the dynamics of plasmas in flames. For the uncertainty quantification (UQ), 22 uncertain reaction rate parameters are selected based on their involvement (i.e. production and consumption channels) in the reaction flow pathways pertaining to the QoIs. This greatly reduces the number of uncertain parameters and thus makes the UQ analysis computationally feasible. The uncertain reaction rate parameters are assumed to follow a uniform distribution with corresponding uncertainties extracted from existing literature (e.g. [3,4,5]). The NISP approach produces the polynomial chaos (PC) representation of the QoIs, which can then be used as a surrogate for the full model, thus enabling efficient sampling for the purpose of inference or sensitivity analysis. However, in the original full-quadrature-based NISP method, the number of realizations of the deterministic solver scale exponentially with the number of stochastic dimensions (i.e. uncertain parameters). To mitigate the high computational cost associated with the NISP method, we employ a recently developed adaptive pseudo-spectral algorithm (based on a direct application of Smolyak's sparse grid formula [6]), which allows for the use of arbitrary admissible sparse grids. Global sensitivity indices enable us to assess the contribution of each of the random inputs to the model variability. Results indicate that

almost all the QoIs are highly sensitive to only a few key reaction rate parameters, including the well-known chemi-ionization reaction CH + O = E- + HCO+.

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Poster 27.

Authors: H. Arda Ülkü, Hakan Bağcı, Eric Michielssen

Title: Explicit MOT Solution of the Mixed-Discretized Time Domain Magnetic Field Integral Equation at Low Frequencies

Abstract: An explicit marching on-in-time (MOT) scheme for solving the mixed discretized time domain magnetic field integral equation is presented. The proposed scheme uses Rao-Wilton-Glisson and Buffa-Christiansen functions as spatial basis and testing functions (mixed spatial discretization) and a $PE(CE)^m$ type predictor-corrector scheme for time marching. Under low frequency excitation (i.e., when the time step is large), mixed discretization scheme ensures the accuracy of the solution while the explicit scheme ensures the efficiency of the MOT.

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Poster 28.

Authors: Kostyantyn Sirenko, Hakan Bağcı

Title: Accurate Simulation of Electromagnetic Transients on 3D Diffraction Gratings

Abstract: A time domain discontinuous Galerkin finite element method with exact absorbing boundary conditions (EACs) for highly-accurate simulation of transient electromagnetic wave interactions on 3D diffraction gratings is presented. EACs when enforced together with periodic boundary conditions permit the truncation of the infinite physical domain of the gratings to a bounded computation domain without introducing any additional errors. Numerical results demonstrate that discretization error of the EACs matches the error of the method used of discretizing the Maxwell equations, and therefore suggest that EAC-based truncation might result in more accurate and/or efficient simulations when compared to PML-based truncation.

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Poster 29.

Authors: Ahmed Al-Jarro, Saber Feki, Hakan Bağcı

Title: OpenACC Implementation of an Explicit Time Domain Volume Integral Equation Solver on a GPU

Abstract: An implementation of an explicit time domain volume integral equation (TD-VIE) solver fine-tuned for efficient execution on graphics processing units (GPUs) is described. The implementation makes use of the OpenACC application program interface (API), which is based on a collection of compiler directives, for the ease of code porting onto the GPU environment. The resulting (serial) implementation runs up to 50 times faster than the original (serial) implementation of the solver developed for the CPU environment.

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Poster 30.

Authors: Yifei Shi, Hakan Bağcı, Mingyu Lu

Title: On the Internal Resonant Modes in Marching-on-in-Time Solution of the Time Domain Electric Field Integral Equation

Abstract: Internal resonant modes are always observed in the marching-on-in-time (MOT) solution of the time domain electric field integral equation (EFIE), although "relaxed initial conditions," which are enforced at the beginning of time marching, should in theory prevent these spurious modes from appearing. It has been conjectured that, numerical errors built up during time marching establish the necessary initial conditions and allow the incident field to induce the internal resonant modes. However, this conjecture has never been proved by systematic numerical experiments. Our numerical results in this paper demonstrate that, the internal resonant modes' amplitudes are indeed dictated by the numerical errors and the spectrum of the incident field. Additionally, it is shown that in a few cases, the internal resonant modes can be made "invisible" by significantly suppressing the numerical errors. These tests prove the conjecture that the internal resonant modes are induced by numerical errors when the time domain EFIE is solved by the MOT method.

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Poster 31

Author: Kody Law

Title: Evaluating Data Assimilation Algorithms

Abstract: Inexpensive data assimilation algorithms are evaluated in comparison with the posterior distribution obtained with a function-space MCMC method, for a well-defined problem with a perfect model. The methods are based on Gaussian approximations and become inaccurate as the non-linearity of the underlying system is increased. They can be modified to give stable estimates of the mean if the true posterior is stable, but such modification typically involves increasing the covariance, leading to a worse estimate of the uncertainty for the original well-defined problem.

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8. SOCIAL PROGRAM:

The workshop offered variety of networking events, including the Welcome Reception Poster Area, the KAUST Dinner, the Thuwal Dinner, morning & afternoon breaks and lunches. The participants have taken the advantage of these opportunities to meet face-to-face with world-class researchers, key decision makers and technical innovators in both industry and academia.