CSE15 Abstracts

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form. A higher-order RK time discretization treats diffusion terms implicitly, so the overall algorithm is limited only by the advection term explicit CFL constraint, regardless of small cells. Accuracy and stability are demonstrated with several simple tests.

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MS157

A Mixed Explicit Implicit Time Stepping Scheme for Cartesian Embedded Boundary Meshes

We present a mixed explicit implicit time stepping scheme for solving the advection equation on Cartesian embedded boundary meshes. The implicit scheme is used to overcome the small cell problem and ensure stability at the cut cells. It is coupled to a standard explicit scheme which is used over most of the mesh. We present a theoretical result about the coupling, and show numerical results in one and more dimensions.

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MS157

Inverse Lax-Wendroff Procedure for Numerical Boundary Conditions of Hyperbolic Equations

We develop a high order finite difference numerical boundary condition for solving hyperbolic Hamilton-Jacobi equations and conservation laws on a Cartesian mesh. The challenge results from the wide stencil of the interior high order scheme and the fact that the boundary may not be aligned with the mesh. Our method is based on an inverse Lax-Wendroff procedure for the inflow boundary conditions. Extensive numerical examples are provided to illustrate its good performance of our method. This is a joint work with Ling Huang and Mengping Zhang, and with Sirui Tan and Francois Vilar.

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MS158

Sequentially Constrained Monte Carlo

Constraints in the parameter or model space typically make sampling from distributions more complex (although more interpretable) than their unconstrained counterparts. We define a Sequentially Constrained Monte Carlo algorithm connecting a simple distribution, to the target distribution by a path defined by the strictness of constraint enforcement. We show general applicability by expanding the usual definition of constraints to include adherence to a theoretical model governed by differential equations.

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MS158

On the Use of Particle Based Methods for the Real Time Identification and Control of Nonlinear Dynamical Systems

The field of structural dynamics is inherently related to the simulation, identification and control of structural systems. This task is not a straightforward one; firstly, due to potential nonlinear behavior; and secondly, due to uncertainties relating to erroneous modeling assumptions, imprecise sensory information, ageing effects, varying loads, and lack of a priori knowledge of the system itself. This talk discusses the implementation of methodologies capable of successfully simulating such systems by encompassing the aforementioned complexities.

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Bayesian Uncertainty Quantification and Propagation for Molecular Dynamic Simulations in Nanoscale Fluid Mechanics

For five decades, molecular dynamics (MD) simulations, in synergy with experiments, have elucidated critical mechanisms in a broad range of physiological systems and technological innovations. However, in nanofluidics, the results of experiments and MD simulations may differ by several orders of magnitude. We show that experimental and large scale MD investigations can be consolidated through a Bayesian framework. Our findings indicate that it is essential to revisit MD simulations in the context of uncertainty quantification.

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MS158

Computationally Efficient Tools for Bayesian Uncertainty Quantification and Propagation in Structural Dynamics

Bayesian uncertainty quantification, including Bayesian hierarchical modelling, are becoming standard tools in structural dynamics for model selection, model parameter calibration, uncertainty propagation and SHM using vibration measurements. For complex linear/nonlinear models, the computations involved in Bayesian asymptotic approximations and MCMC sampling tools may be excessive. Drastic reduction in computational effort in model intrusive and/or non-intrusive schemes is achieved by integrating model reduction techniques, adjoint methods, surrogate models, parallel computing and highly-parallelizable sampling schemes. Acknowledgement: This research has been implemented under the ARISTEIA Action of the Operational Programme Education and Lifelong Learning and was co-funded by the European Social Fund (ESF) and Greek National Resources.

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H-Matrix Accelerated Second Moment Analysis for Potentials with Rough Correlation

We consider the efficient solution of strongly elliptic potential problems with stochastic Dirichlet data by the boundary integral equation method. The computation of the solutions two-point correlation is well understood if the two-point correlation of the Dirichlet data is known and sufficiently smooth. Unfortunately, the problem becomes much more involved in case of rough data. We will show that the concept of the H-matrix arithmetic provides a powerful tool to cope with this problem. By employing a parametric surface representation, we end up with an H-matrix arithmetic based on balanced cluster trees. This considerably simplifies the implementation and improves the performance of the H-matrix arithmetic. Numerical experiments are provided to validate and quantify the presented methods and algorithms.

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MS159

Adaptive Monte Carlo and Quasi-Monte Carlo Integration

Monte Carlo methods are used for computing means of random variables with complex distributions. Both Monte Carlo methods and quasi-Monte Carlo methods are also used for computing high dimensional integrals. A key question in these computations is when to stop, while ensuring that the desired accuracy is obtained. Adaptive (quasi-)Monte Carlo algorithms rely on data-based error bounds to answer this question. This talk describes recent work to construct such error bounds and ensure that they are trustworthy. We also derive upper bounds on the computational costs of our adaptive algorithms. A key idea is to consider cones of random variables or integrands. Our new algorithms have been implemented in the Guaranteed Automatic Integration Library (GAIL) https://code.google.com/p/gail/.

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MS159

Application of Quasi-Monte Carlo Methods to PDEs with Random Coefficients

PDEs with random coefficients are an important source of high dimensional problems. One example is the flow through porous medium: because of the near impossibility of modeling the microscopic channels through which water can flow in a porous layer, it is common engineering practice to model the porous medium as a random permeability field. The quantity of interest is therefore an expected value with respect to the random field, leading to a high dimensional integral where the number of variables is as high as the number of parameters needed to model this random field (it can be infinite). In this talk I will explain how quasi-Monte Carlo (QMC) methods can be tailored to a prototype of such integrals. I will discuss the fast construction of higher order QMC methods to improve the convergence rate and the use of multi-level techniques to improve the computational cost. The talk will touch on a number of joint works with Ivan Graham and Rob Scheichl (Bath), Dirk Nuyens (KU Leuven), Christoph Schwab (ETH Zurich), and Ian Sloan, James Nichols, Josef Dick and Quoc Le Gia (UNSW).

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