DVR 0065528

Programme on

"Numerical Analysis of Complex PDE Models in the Sciences"

June 11 – August 17, 2018

organized by

Annalisa Buffa (EPFL Lausanne), Thomas Y. Hou (Caltech), J. Markus Melenk (TU Vienna), Ilaria Perugia (U Vienna), Christoph Schwab (ETH Zurich)

Workshop 2 on

"Interplay of multiscale data assimilation and data science with advanced PDE discretizations"

June 25 – 29, 2018

organized by

Thomas Y. Hou (Caltech) and J. Markus Melenk (TU Vienna)

Abstracts

Assyr Abdulle (EPFL)

Bayesian multiscale inverse problems and probabilistic numerical methods

Abstract: In this talk we discuss several challenges that arise when solving inverse problems using Bayesian techniques. The numerical solvers used to compute the forward model of such problems induce a propagation of the discretization error into the posterior measure for the parameters of interest. This uncertainty originating from the numerical approximation error can be accounted for using probabilistic numerical methods. New probabilistic numerical methods for ordinary differential equations (ODEs) that share geometric properties of the true solution will be presented in the first part of this talk and we will comment on these techniques for partial differential equations (PDEs).
In the second part of the talk, we will discuss inverse problems form PDEs which vary on a very fine scale ε using Bayesian techniques. We propose a new strategy based on a homogenized forward model. Using G-convergence, we show that true posterior converges to the "homogenized posterior" in the Hellinger metric as $\varepsilon \to 0$. We then propose a numerical technique based on numerical homogenization and reduced basis techniques for a cheap evaluation of the forward model in a Markov Chain Monte Carlo procedure. We also comment on a procedure to account for the modeling error at fixed ε.

References:

A. Abdulle, G. Garegnani, Random time step probabilistic methods for uncertainty quantification in chaotic and geometric numerical integration, *Preprint* (2017).
A. Abdulle, G. Garegnani, Probabilistic geometric integration of Hamiltonian systems based on random time steps, *Preprint* (2018).
A. Abdulle, A. Di Blasio, Numerical homogenization and model order reduction for multiscale inverse problems, submitted to publication, *Preprint* (2017).

A. Abdulle, A. Di Blasio, A Bayesian numerical homogenization method for elliptic multiscale inverse problems, *Preprint* (2018).

Michal Branicki (University of Edinburgh & The Alan Turing Institute, UK)

Accuracy of a class of nonlinear filters for dissipative PDEs in the presence of model error

Abstract: We consider the filtering problem for estimating dissipative PDE dynamics with linear observations where the optimal estimate is given w.r.t. the quadratic cost function. The filter equations are derived by exploiting connections to a dual stochastic control problem. In particular, this approach provides a framework for a systematic derivation of suboptimal Bayesian filters with a sequential update on the error covariance. The two-dimensional, incompressible Navier-Stokes equation in a periodic geometry is utilised to illustrate the results with sparse observations aliasing fine-scale information into the assimilation space.

Zhiming Chen (Chinese Academy of Sciences)

The Reverse Time Migration Method for Inverse Scattering Problems

Abstract: The reverse time migration (RTM) or the closely related prestack depth migration methods are nowadays widely used in exploration geophysics. It is originated in the simple setting of the exploding reflector model. For imaging the complex medium in practical applications, the analysis of the migration method is usually based on the high frequency assumption, so that the geometric optics approximation can be used. We report our recent efforts in establishing new mathematical understanding of the RTM method without geometric optics assumption for inverse scattering problems. Our resolution analysis, which applies in both penetrable and non-penetrable obstacles with sound soft or impedance boundary condition on the boundary of the obstacle, implies that the RTM imaging functional always peaks on the boundary of the scatterers. This new mathematical understanding leads to several new direct imaging algorithms including: imaging for electromagnetic objects, imaging in half-space acoustics, imaging in closed waveguide, and imaging for scattering data without phase information. In this talk we will report the ideas of the RTM method and our recent result for imaging extended scatterers in the half-space and imaging scatterers using only phaseless scattering data. This talk is based on joint works with Junqing Chen and Guanghui Huang.

Eric Chung (The Chinese University of Hong Kong)

Generalized multiscale finite element methods and nonlocal multi-continua upscaling for heterogeneous and fracture media

Abstract: In this talk, we present the Constraint Energy Minimizing Generalized Multiscale Finite Element Method (CEM-GMsFEM). The main goal of this work is to design multiscale basis functions within GMsFEM framework such that the convergence of method is independent of the contrast and linearly decreases with respect to mesh size if oversampling size is appropriately chosen. We would like to show a mesh-dependent convergence with a minimal number of basis functions and an assumption that the oversampling size weakly depends on the contrast. In addition, we present a rigorous and accurate non-local (in the oversampled region) upscaling framework. Our proposed method consists of identifying multi-continua parameters via local basis functions and constructing non-local (in the oversampled region) transfer and effective properties. To achieve this, we derive appropriate local

problems in oversampled regions. Finally, we present numerical results, which show that the proposed approaches can provide good accuracy. This work is partially supported by the Hong Kong RGC GRF (Project: 14317516).

Yalchin Efendiev (Texas A&M University)

Data Integration in Multiscale Simulations

Abstract: In this talk, I will discuss several data integration techniques in multiscale simulations. I will give a brief overview of multiscale simulation concepts that will be used. These multiscale techniques are designed for problems when the coarse grid does not resolve scales and contrast. I will describe the relation between multiscale and upscaling methods. I will describe three data integration techniques. The first one, Bayesian multiscale modeling, will sample basis functions and incorporate available data. In the second approach, we will use deep learning techniques to design and modify existing multiscale methods in the presence of data and nonlinearities. Finally, I will talk about generalized multiscale inversion algorithms.

Bjorn Engquist (University of Texas at Austin)

Sampling and low rank compression of multiscale functions and operators

Abstract: Information theory dictates that for band limited multiscale functions at least two samples per wavelength are required to fully recover the original signals. We will discuss upper and lower bounds for the sampling rate when more than just the band limits are known. This is a natural background for potential discretization strategies regarding numerical approximations of differential equation. For discrete operators approximating multiscale problems the focus will be on low rank compression, which often is the basis for fast algorithms. The elliptic cases are quite well understood but problems with oscillatory kernels are more challenging. Frequency domain wave equations are examples for which elliptic style compression in fast multipole methods, H-matrix techniques and preconditioning must be modified. We will give upper and lower bounds for possible low rank compression based on Greens function decorrelation.

Dimitris Giannakis (New York University)

Data-driven approaches for spectral decomposition of ergodic dynamical systems

Abstract: We discuss techniques for approximating the spectra of Koopman operators governing the evolution of observables in ergodic dynamical systems. These methods are based on representations of Koopman operators in bases for appropriate Hilbert spaces of observables learned from time-ordered measurements of the system using kernel algorithms for machine learning. We establish spectral convergence results for the point spectrum, and present regularization approaches applicable to systems with continuous spectra. We illustrate this framework with applications to toy dynamical systems and climate data.

Viet-Ha Hoang (Division of Mathematical Sciences, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore)

Bayesian inverse homogenization

Abstract: We consider the problem of recovering the microstructure of a locally periodic multiscale medium, given limited noisy observations on the solution of a multiscale elliptic equation governing a physical process in the medium. We determine the types of observations that give us the desired information on the multiscale coefficient. We then discuss some computational issues on sampling the posterior measure on the space of locally periodic coefficients.

Thomas Hou (Caltech)

Sparse Operator Compression for Higher Order Elliptic PDEs and Graph Laplacians with Rough Coefficients

Abstract: We introduce the sparse operator compression to compress a self-adjoint higher order elliptic operator with rough coefficients and various boundary conditions. The operator compression is achieved by using localized basis functions, that are energy minimizing functions on local patches. On a regular mesh with mesh size h, the localized basis functions have supports of diameter $O(hlog(1/h))$, and give optimal compression rate of the solution operator. We show that our method achieves the optimal compression rate of the solution operator. We then discuss how to generalize this operator compression to develop a fast solver for graph Laplacians with rough coefficients using a novel energy decomposition method. This decomposition framework naturally reflects the intrinsic geometric information of the operator that inherits the localities of the topological structure. Utilizing this information, we propose a multiresolution operator compression scheme for the inverse operator of a symmetric positive definite matrix with controllable compression error and condition number. This is a joint work with Pengchuan Zhang, De Huang, and Ka Chun Lam.

Lise-Marie Imbert-Gérard (University of Maryland)

Wave propagation in inhomogeneous media: Beyond the Helmholtz equation

Abstract: Trefftz methods rely, in broad terms, on the idea of approximating solutions to PDEs using basis functions which are exact solutions of the Partial Differential Equation (PDE), making explicit use of information about the ambient medium. But wave propagation problems in inhomogeneous media is modeled by PDEs with variable coefficients, and in general no exact solutions are available. Generalized Plane Waves (GPWs) are functions that have been introduced, in the case of the Helmholtz equation with variable coefficients, to address this problem: they are not exact solutions to the PDE but are instead constructed locally as high order approximate solutions. We will discuss the extension of the GPW construction to other equations, like the mild-slope equation in two dimensions and the convected Helmholtz equation in three dimensions.

Barbara Kaltenbacher (Alpen-Adria-Universität Klagenfurt)

Adaptive discretization of inverse problems based on functional error estimators

Abstract: (joint work with Christian Clason, University of Duisburg-Essen, Daniel Wachsmuth, University of Würzburg, and Mario Luiz Previatti de Souza, Alpen-Adria-Universität Klagenfurt)

So-called functional error estimators (Repin, 2000) provide a valuable tool for reliably estimating the discretization error for a sum of two convex functions. We apply this concept to Tikhonov regularization for the solution of inverse problems for partial differential equations, not only for quadratic Hilbert space regularization terms but also for nonsmooth Banach space penalties. Examples include the measure-space norm (i.e., sparsity regularization) or the indicator function of an L^∞ ball (i.e., Ivanov regularization). The error estimators can be written in terms of residuals in the optimality system that can then be estimated by conventional techniques, thus leading to explicit estimators. This is illustrated by means of an elliptic inverse source problem with the above-mentioned penalties, and numerical results are provided for the case of sparsity regularization.

Andrea Moiola (Dipartimento di Matematica, Universita di Pavia)

Scattering by fractal screens: functional analysis and computation

Abstract: The mathematical analysis and numerical simulation of acoustic and electromagnetic wave scattering by planar screens is a classical topic. The standard technique involves reformulating the problem as a boundary integral equation (BIE) on the screen, which can be solved numerically using a boundary element method (BEM). Theory and computation are both well-developed for the case where the screen is an open subset of the plane with smooth (e.g. Lipschitz or smoother) boundary. In this talk I will explore the case where the screen is an arbitrary subset of the plane; in particular, the screen could have fractal boundary, or itself be a fractal. Such problems are of interest in the study of fractal antennas in electrical engineering, light scattering by snowflakes/ice crystals in atmospheric physics, and in certain diffraction problems in laser optics. The roughness of the screen presents challenging questions concerning how boundary conditions should be enforced, and the appropriate function space setting. But progress is possible and there is interesting behaviour to be discovered: for example, a sound-soft screen with zero area (planar measure zero) can scatter waves provided the fractal dimension of the set is large enough. This research has also motivated investigations into the properties of fractional Sobolev spaces (the classical Bessel potential spaces) on non-Lipschitz domains. Accurate computations are also challenging because of the need to adapt the basis functions to the fine structure of the fractal. I will present a BEM convergence theory together with numerical results and outline some outstanding open questions. This is joint work with Simon Chandler-Wilde (Reading) and David Hewett (UCL).

Peter Monk (University of Delaware, USA)

Optimal design of thin film solar cells

Abstract: The optimal design of thin film solar cells requires modeling of both 1) the absorption of solar light and 2) the flow of currents throughout the device. The goal is to maximize the efficiency of the device by ensuring the optical and electrical behaviors complement one another. Because of the presence of local maxima in the figure efficiency (our figure–of–merit), we choose to search for an optimal design using a population based stochastic search technique called the Differential Evolution Algorithm. This algorithm requires a large number of evaluations of the figure–of–merit functional to achieve a reliable estimate of the optimal state, but no derivative information is needed. In addition, the figure–of–merit may need to be evaluated for widely different device configurations. These requirements have influenced our modeling choices.
For the optical modeling, we need to solve Maxwells equations across a wide range of wavelengths throughout the visible solar spectrum in order to predict the generation rate of free electrons. We use a Fourier based technique with a special solver, called the Rigorous Coupled Wave Analysis (RCWA) method. This method is fast and does not require remeshing between solar cells with different geometrical structures. The output from RCWA is used as a source term in the electrical model, driving the flow of electrons and holes in semiconductor elements of the device. This electronic behaviour is modeled using the classical drift-diffusion equations, which are approximated

using the Hybridizable Discontinuous Galerkin (HDG) method. This formulation naturally allows upwinding and the handling of heterojunctions. I shall describe each component of the model, giving numerical results, and show how we can achieve a successful optimal design process.

Mario Ohlberger (Applied Mathematics Münster)

Localized Model Reduction for PDE-constrained Parameter Optimization

Abstract: We will address model order reduction for parameterized multiscale or large scale problems, where traditional projection based model order reduction methods fail due to enormous or even prohibitive computational “offline”-costs. In such situations localized model reduction methods based on localized training (BEOR17, BS18) and online enrichment (OS15) are particularly promising. In this contribution, we demonstrate recent advances of localized reduced basis methods in the context of PDE constrained optimization and inverse problems (OSS18). In particular, we will present localized true error estimates for the optimization problem, including a posteriori error estimates for the objective functional and the optimal parameters or parameter functions, and numerical experiments to demonstrate the potential of our approach. The numerical results were obtained with the newly developed model reduction algorithms implemented in pyMOR (see http://pymor.org and MRS2016).

References:

BS18: A. Buhr and K. Smetana. Randomized local model order reduction. Technical report, arXiv:1706.09179, preprint (submitted), 2017.
BEOR17: A. Buhr, C. Engwer, M. Ohlberger, and S. Rave. ArbiLoMod, a Simulation Technique Designed for Arbitrary Local Modifications. SIAM J. Sci. Comput., 39(4):A1435A1465, 2017.
MRS2016: R. Milk, S. Rave, F. Schindler. pyMOR- generic algorithms and interfaces for model order reduction. SIAM J. Sci. Comput. 38(5):S194–S216, 2016.
OSS18: M. Ohlberger, M. Schaefer, and F. Schindler. Localized model reduction in pde constrained optimization. Accepted for publication in: Procceedings of the DFG-AIMS Workshop on Shape optimization, homogenization and control, AIMS Sngal, Mbour, Sngal. 2017.
OS15: M. Ohlberger, F. Schindler. Error control for the localized reduced basis multi-scale method with adaptive on-line enrichment. SIAM J. Sci. Comput. 37(6):A2865–A2895, 2015.

Sergei Pereverzyev (Johann Radon Institute for Computational and Applied Mathematics (RICAM), Austrian Academy of Sciences)

Application of graph Laplacian in semi-supervised learning

Abstract: The problem of semi-supervised learning by Tikhonov regularization method in Reproducing Kernel Hilbert Spaces (RKHS) is considered. We propose a new technique for constructing a reproducing kernel directly from given data. This technique is based on a technology of spectral graph theory. We use the eigenvectors of the graph Laplacian to mimic the geometry of underlying manifold that is usually unknown. In contrast to existing approaches, we construct a data-dependent kernel that directly generates RKHS. The adaptive approach to the choice of regularization parameters is also presented. We verified the proposed method on well-known examples (including two- and tree-moons data sets) and also applied it to the problem of automatic gender identification.

Daniel Peterseim (Universität Augsburg)

Quasi-local numerical stochastic homogenization

Abstract: This talk proposes a numerical upscaling procedure for elliptic boundary value problems with diffusion tensors that vary randomly on small scales. The method compresses the random partial differential operator to an effective deterministic operator that represents the expected solution on a coarse scale of interest. The effective operator is quasi-local in the sense that its integral kernel decays exponentially fast and, hence, admits a sparse representation. Error estimates consisting of a priori and a posteriori terms are provided that allow one to quantify the impact of microscopic uncertainty on expected effective responses.

Sebastian Reich (University of Potsdam and University of Reading)

Data assimilation: Coupling of probability measures

Abstract: Ensemble-based assimilation of data into evolutionary models, either in the form of SDEs or PDEs, can be seen as introducing interacting particle approximations to time evolving probability measures conditioned on the data. Since Bayes formula only provides information at the level of conditioned probability measures, interacting particle approximations require to couple those measures in an appropriate manner. In this talk, such couplings will be discussed from the perspective of optimal transportation and Schrdinger systems and will be put into the perspective of existing ensemble data assimilation methods.

Gianluigi Rozza (SISSA, International School for Advanced Studies, Mathematics Area, mathLab, Trieste, Italy)

Reduced Order Methods: state of the art and perspectives with a special focus on Computational Fluid Dynamics

Abstract: In this talk, we provide the state of the art of Reduced Order Methods (ROM) for parametric Partial Differential Equations (PDEs), and we focus on some perspectives in their current trends and developments, with a special interest in parametric problems arising in offline-online Computational Fluid Dynamics (CFD). Systems modelled by PDEs are depending by several complex parameters in need of being reduced, even before the computational phase in a pre-processing step, in order to reduce parameter space. Efficient parametrizations (random inputs, geometry, physics) are very important to be able to properly address an offline-online decoupling of the computational procedures and to allow competitive computational performances. Current ROM developments in CFD include: a better use of stable high fidelity methods, considering also spectral element method, to enhance the quality of the reduced model too; more efficient sampling techniques to reduce the number of the basis functions, retained as snapshots, as well as the dimension of online systems; the improvements of the certification of accuracy based on residual based error bounds and of the stability factors, as well as the the guarantee of the stability of the approximation with proper space enrichments. For nonlinear systems, also the investigation on bifurcations of parametric solutions are crucial and they may be obtained thanks to a reduced eigenvalue analysis of the linearised operator. All the previous aspects are very important in CFD problems to be able to focus in real time on complex parametric industrial and biomedical flow problems, or even in a control flow setting, and to couple viscous flows - velocity, pressure, as well as thermal field - with a structural field or a porous medium, thus requiring also an efficient reduced parametric treatment of interfaces between different physics. Model flow problems will focus on few benchmark cases in a time-dependent framework, as well as on simple fluid-structure interaction problems or flow control problems in environmental sciences or medicine. Further examples of applications will be delivered concerning shape optimisation applied to industrial problems.

Stefan Sauter (Institut für Mathematik, Universität Zürich)

Estimating the effect of data simplification for elliptic PDEs

Abstract: In many cases, the numerical simulation of complicated physical phenomena consists of various modelling and discretization steps. This includes data simplification (replacing complicated coefficients by simpler ones, using dimension-reduced models, applying homogenization models) and the numerical discretization. In many cases the final approximation is constructed by combining solutions of simpler problems in a sophisticated way via a postprocessing step.
The a priori and a posteriori analysis for such types of problems typically require some regularity of the simplified problems. In particular, for the a posteriori error analysis the (estimated) value of the regularity constant (of the simplified problem) with respect to a $W^{1,p}$ norm for some $p > 2$ is required.
In our talk, we will present model problems where the a posteriori analysis leads to such regularity problems and explain theoretical tools for their estimation.

Otmar Scherzer (University of Vienna)

On a multi-level algorithms for solving the inverse boundary value problem for the Helmholtz equation.

Abstract: We study the inverse boundary value problem for the Helmholtz equation using the Dirichlet-to-Neumann map at selected frequencies as the data. A conditional Lipschitz stability estimate for the inverse problem holds in the case of wavespeeds that are a linear combination of piecewise constant functions (following a domain partition) and gives a framework in which the numerical scheme for the inverse problem converges. The stability constant grows exponentially as the number of subdomains in the domain partition increases. We establish an order optimal upper bound for the stability constant. We eventually realize computational experiments. This is joint work with Elena Beretta (Milan), Florian Faucher (INRIA), and Maarten De Hoop (RICE).

Claudia Schillings (University of Mannheim)

Well-posedness and convergence analysis of the ensemble Kalman inversion

Abstract: The Ensemble Kalman filter (EnKF) has had enormous impact on the applied sciences since its introduction in the 1990s by Evensen and coworkers. It is used for both data assimilation problems, where the objective is to estimate a partially observed time-evolving system, and inverse problems, where the objective is to estimate a (typically distributed) parameter appearing in a differential equation. In this talk we will focus on the identification of parameters through observations of the response of the system - the inverse problem. The EnKF can be adapted to this setting by introducing artificial dynamics. Despite documented success as a solver for such inverse problems, there is very little analysis of the algorithm. In this talk, we will discuss well-posedness and convergence results of the EnKF based on the continuous time scaling limits, which allow to derive estimates on the long-time behavior of the EnKF and, hence, provide insights into the convergence properties of the algorithm. This is joint work with Dirk Bloemker (U Augsburg), Andrew M. Stuart (Caltech), Philipp Wacker (FAU Erlangen-Nürnberg) and Simon Weissmann (U Mannheim).

Joachim Schöberl (TU Vienna)

Hybrid mixed methods for the Helmholtz equation

Abstract: We present a hybrid mixed method for the heterogeneous Helmholtz equation. After static condensation, the remaining facet variables are left and right going impedance traces. We show h-version error estimates, and prove conservation of energy in a proper sense. The main advantage of the method is to be solver-friendly: Simple block-preconditioners within three-term Krylov-space methods lead to convergent methods. Numerical examples formulated within the Python interface of NGSolve are presented.

Zuoqiang Shi (Tsinghua University)

PDE-based models in learning manifold

Abstract: Manifold is very powerful to model the low dimensional structure hidden in high dimensional data. In this talk, I will introduce several PDE-based model to study the interpolation problem on the manifold. We will reveal the close connections between PDEs and some deep neural networks. Theoretical analysis and numerical simulations show that PDEs provide us powerful tools to understand high dimensional data.

Benjamin Stamm (RWTH Aachen University)

An embedded corrector problem for stochastic homogenization

Abstract: In this talk, we present a new embedded corrector problem in the context of stochastic homogenisation problems. The main idea is to not truncate the computational domain and consider a sequence of increasing bounded domains on which the corrector problem is solved. Instead, the approach is based on truncating the oscillating coefficient by a specific constant value on the outside of a sequence of increasing bounded domains and referring to integral equations to solve the modified corrector problem on the entire unbounded domain. After presenting the theoretical results, we will present a Galerkin discretisation of the integral equation to approximate the effective coefficients in stochastic homogenization for random media with spherical inclusions and illustrate how the fast multipole method (FMM) can be employed to obtain a numerical method that scales linearly with the number of spherical inclusions. Some numerical test cases will illustrate the behaviour of this method.

Andrew Stuart (Caltech)

Large Graph Limits of Learning Algorithms

Abstract: Many problems in machine learning require the classification of high dimensional data. One methodology to approach such problems is to construct a graph whose vertices are identified with data points, with edges weighted according to some measure of affinity between the data points. Algorithms such as spectral clustering, probit classification and the Bayesian level set method can all be applied in this setting. The goal of the talk is to describe these algorithms for classification, and analyze them in the limit of large data sets. Doing so leads to interesting problems in the calculus of variations, in stochastic partial differential equations and in Monte Carlo Markov Chain, all of which will be highlighted in the talk. These limiting problems give insight into the structure

of the classification problem, and algorithms for it.
Collaboration with: Andrea Bertozzi (UCLA), Michael Luo (UCLA), Kostas Zygalakis (Edinburgh), Matt Dunlop (Caltech), Dejan Slepcev (CMU), Matt Thorpe (Cambridge), Victor Chen (Caltech), Omiros Papaspiliopoulos (UPF-Barcelona)
https://arxiv.org/abs/1703.08816
https://arxiv.org/abs/1703.08816

Barbara Verfürth (University of Münster)

Numerical multiscale methods for Maxwellß equations in complex media

Abstract: The propagation of electromagnetic fields in heterogeneous materials is considered with growing interest as some of these media show unusual behavior, such as frequency band gaps and even negative refraction. To produce such effects, the materials possess some (mostly periodic) sub-wavelength fine-scale structures, possibly even with a high contrast between at least two composites.
The simulation of such problems is quite challenging due to the general wave nature of the problem and the additional fine-scale oscillations from the material inhomogeneities. At the example of the time-harmonic Maxwell's equations, we show that a (fine-scale) corrector is needed for a good approximation in L^2. We discuss how this corrector can be efficiently computed as the solution of local cell problems. We present corresponding numerical multiscale methods and their a priori error analysis.
Numerical examples conform the theoretical results and illustrate some of the interesting physical phenomena. For instance, a high contrast between two composites in a periodic microstructure can lead to frequency band gaps caused by (Mie) resonances.

Gilles Vilmart (University of Geneva)

Uniformly accurate numerical schemes for highly oscillatory evolution problems

Abstract: We introduce a new methodology to design uniformly accurate methods for evolution problems that are oscillatory in time. The targeted models are envisaged in a wide spectrum of regimes, from nonstiff to highly oscillatory. Thanks to an averaging transformation, the stiffness of the problem is softened, allowing for standard schemes to retain their usual orders of convergence. High-order numerical approximations with favourable geometric properties are obtained, with errors and cost that are independent of the regime.
This talk is based on a joint work with Philippe Chartier, Mohammed Lemou, and Florian Mhats (Rennes).
Preprints available at http://www.unige.ch/~vilmart.

Jonathan Weare (University of Chicago)

Stratification for Markov Chain Monte Carlo Simulation

Abstract: I will discuss a Monte Carlo approach to computing statistical averages that is based on a decomposition of the target average of interest into subproblems that are each individually easier to solve and can be solved in parallel. It is a close relative of the classical stratified sampling approach that has long been a cornerstone of experimental design in statistics. The most basic version of the scheme computes averages with respect to a given density and is a generalization of the umbrella sampling method for the calculation of free energies. For this scheme we

have developed error bounds that reveal that the existing understanding of umbrella sampling is incomplete and potentially misleading. We demonstrate that the improvement from umbrella sampling over direct simulation can be dramatic in certain regimes. Our bounds are motivated by new, more detailed perturbation bounds for stochastic matrices. Finally, I will show an application of umbrella sampling and a tempering variant of umbrella sampling in the estimation of cosmological constraints from supernova data.
