# EPSRC Symposium Workshop - Multiscale Systems: Theory and Applications

## Abstracts

**Nils Berglund** (Orleans)

*Canards, mixed-mode oscillations and interspike distributions in stochastic systems*

Mixed-mode oscillations (MMOs) are patterns of alternating large and small-amplitude oscillations which occur in applications ranging from chemical reactions and neuronal dynamics to climate models. We will discuss two different mechanisms by which noise can modify mixed-mode patterns. The first one applies to excitable systems operating near a singular Hopf bifurcation, where noise can induce MMOs which are absent in the determinisic case. Characterising the mixed-mode patterns as a function of noise intensity yields for instance information on the interspike interval statistics in the stochastic FitzHugh-Nagumo equations. The second mechanism concerns systems with one fast and two slow variables admitting a folded-node singularity. In that case, MMOs are already present in the absence of noise, and are related to so-called canard solutions. Additive noise modifies the mixed-mode patterns by blurring small-amplitude oscillations and by causing early transitions.

Based on joint work with Barbara Gentz (Bielefeld), Christian Kuehn (Vienna) and Damien Landon (Orléans).

**Dirk Blömker** (Augsburg)

*Stabilization due to additive noise*

We consider a stochastic partial differential equation near a change of stability. Here the evolution of solutions is dominated by the modes (or eigenfunctions) changing stability. Using the natural separation of time-scales the dominant behaviour is well described by the so called amplitude equation. Non-degenerate noise not directly acting on the dominant modes can nevertheless have an impact due to nonlinear interaction. As an example we discuss the Swift-Hohenberg equation, where noise can lead to stabilization or destabilization in the dynamics.
This is joint work with Konrad Klepel and Wael Mohammed.

**Gero Friesecke** (TU Munich)

*Multiscale aspects of electronic structure: analysis, model reduction, applications*

In electronic structure theory, a unifying and accurate mathematical model is available, namely the (nonrelativistic, Born-Oppenheimer) electronic Schrödinger equation. However, to understand and efficiently simulate electronic structure, one has to face two major challenges: First, high-dimensionality. The Schrödinger eq. for a molecule with N electrons is a PDE in 3N dimensions. Thus the equation for a single Carbon atom (N=6) on a coarse ten point grid in each direction (K=10) already has a prohibitive 10^18 degrees of freedom. Second, one is dealing with a tough multiscale problem. The electronic state of a particular system, and hence its chemical behaviour, is not governed by total energies (mathematically: eigenvalues of the PDE), but small energy differences between competing states (mathematically: spectral gaps of the PDE). For instance the spectral gap between the two lowest Carbon eigenvalues is only 0.1 percent of the total energy. But this gap is of crucial chemical importance, as the two states have different spin and angular momentum symmetry (^3 P versus ^1 D). If the ordering was switched, Carbon would behave entirely differently, like a transition metal such as Scandium or Yttrium.

In my talk I will try to give an overview over interesting asymptotic limits of the many-electronic Schrödinger equation, and discuss strengths and failures of the ensuing reduced models. Two examples will be considered in more detail: the fixed-N large-Z limit for atoms and its relevance to capture small spectral gaps (joint work with Ben Goddard and Christian Mendl), and the semiclassical limit of the Hohenberg-Kohn density functional and its relevance to capture basic aspects of electron correlation (joint work with Codina Cotar and Claudia Klueppelberg).

References:
G.Friesecke, B.D.Goddard, Asymptotics-based CI models for atoms: properties, exact solution of a minimal model for Li to

Ne, and application to atomic spectra, Multiscale Model. Simul. Vol. 7, No. 4, pp. 1876-1897, 2009
Ch.Mendl, G.Friesecke, Efficient Algorithm for Asymptotics-Based CI and Electronic Structure of Transition Metal Atoms, J. Chem. Phys. 133, 184101, 2010
C.Cotar, G.Friesecke, C.Klüppelberg, Density functional theory and optimal transportation with Coulomb cost, http://arxiv.org/abs/1104.0603, 2011

**Carsten Hartman** (Berlin)

*Steered molecular dynamics: some ideas from robust control*

In the talk I will present some recent developments in robust control of bilinear systems that appear relevant in the context of nonequilibrium molecular dynamics and quantum control. A particular focus is on low-rank approximation techniques that make the calculation of an optimal control numerically feasible.

**Leonid Koralov** (UMD)

*Random, deterministic and nonlinear perturbations of dynamical systems*

In the first part of the talk we discuss deterministic and stochastic perturbations of incompressible flows. Even in the case of purely deterministic perturbations, the long-time behavior of such systems can be stochastic, in a certain sense. The stochasticity is caused by the instabilities near the saddle points of the non-perturbed system as well as by the ergodic components of the flow.
In the second part of the talk we describe the asymptotic behavior of solutions to quasi-linear parabolic equations with a small parameter at the second order term and the long time behavior of corresponding diffusion processes. In particular, we discuss the exit problem and metastability for the processes corresponding to quasi-linear initial-boundary value problems.

**S. Krumscheid** (Imperial)

*Semi-parametric drift and diffusion estimation for multiscale diffusions*

Consider the problem of statistical inference for the effective dynamics of multiscale diffusion processes with (at least) two widely separated characteristic time scales. More precisely, we seek to determine parameters in the effective equation describing the dynamics on the longer diffusive time scale (homogenization framework). We consider the case where both the drift and the diffusion coefficients in the effective dynamics are space-dependent and depend on multiple unknown parameters. It is known that classical estimators, such as Maximum Likelihood and Quadratic Variation of the Path Estimators, fail to obtain reasonable estimates for parameters in the effective dynamics when based on observations of the underlying multiscale diffusion. We propose a novel algorithm for estimating both the drift and diffusion coefficients in the effective dynamics based on a semi-parametric framework. We demonstrate by means of extensive numerical simulations of a number of selected examples that the algorithm performs well when applied to data from a multiscale diffusion. The examples also illustrate that the algorithm can be used effectively to obtain accurate and unbiased estimates.

**Benedict Leimkuhler** (Edinburgh)

*Molecular dynamics, and numerical methods for sampling the Gibbs measure*

Many complex dynamical systems are subject to uncertainty in the initial data, chaotic internal mixing, and unresolved interactions with an environment. For these reasons a statistical perspective is often taken: trajectories are treated as tools for computing averages with respect to some statistical ensemble (defined by a suitable phase space density, typically a function of the energy). 'Thermostats' are (typically) stochastic-dynamical models that facilitate such

calculations. Once a thermostatted system has been defined there is still the challenge of effectively integrating the stochastic differential equations in a robust, efficient manner. For molecular dynamics these requirements are very demanding, since the landscapes involved are very rugged and the cost of computing forces often very high. I will discuss the numerical challenges and describe some innovative methods for the case where only the sampling of the invariant measure is of interest. This talk describes joint work with Charles Matthews.

**Tony Lelièvre** (CERMICS)

*Sampling methods in molecular dynamics*

We will present some mathematical results on numerical methods for efficient sampling in MD, with an emphasis on techniques used to sample trajectories between metastable states. This presentation is based on the following papers:
[1] C. Le Bris, T. Lelièvre, M. Luskin and D. Perez, *A mathematical formalization of the parallel replica dynamics*, http://arxiv.org/abs/1105.4636 .
[2] F. Cérou, A. Guyader, T. Lelièvre and D. Pommier, *A multiple replica approach to simulate reactive trajectories*, Journal of Chemical Physics **134**, 054108, (2011).

**Richard Di Liu** (MSU)

*Numerical methods for stochastic bio-chemical reacting networks with multiple time scales*

Multiscale and stochastic approaches play a crucial role in faithfully capturing the dynamical features and making insightful predictions of cellular reacting systems involving gene expression. Despite their accuracy, the standard stochastic simulation algorithms are necessarily inefficient for most of the realistic problems with a multiscale nature characterized by multiple time scales induced by widely disparate reactions rates. In this talk, I will discuss some recent progress on using asymptotic techniques for probability theory to simplify the complex networks and help to design efficient numerical schemes.

**Peter Moerters** (Bath)

*Ageing in the parabolic Anderson model*

The parabolic Anderson model is the Cauchy problem for the heat equation with random potential. The focus in this talk is on phenomena that are due to a highly irregular potential, which we model by a spatially independent, identically distributed random field with heavy tails. In particular, we show that changes in the shape of the solution become less likely over time and hence the typical time scales of the system are increasing, a phenomenon known as ageing.
The talk is based on joint work with Marcel Ortgiese and Nadia Sidorova.

**Houman Owhadi** (Caltech)

*Geometric numerical integration of multiscale Hamiltonian systems*

This talk will cover three different strategies for the symplectic numerical integration of stiff (multiscale) Hamiltonian ODEs and PDEs.
The first and most general one is based flow averaging via the switching `on' and `off' of stiff coefficients over mesoscopic time-steps (and possibly, space-steps for PDEs). The second one: is designed for high-dimensional systems with slowly varying quadratic stiff potentials, uses macroscopic time-steps, and is based on the introduction of a new symplectic matrix exponentiation scheme. The third one: is designed for the fast symplectic integration of constrained dynamic, uses macroscopic time-steps, and is based on the symplectic linearization of the push-forward of the Newmark family of implicit integrators. This is a joint work with Molei Tao (Caltech) and Jerry Marsden (Caltech).

**Andrey Piatnitski** (Narvik University College)

*Homogenization of spin systems*

The talk will focus on the limit behaviour of surface and line energies defined on lattice (spin) systems in $\mathbb{Z}^d$ through bond interactions. We mostly dwell on nearest neighbors interaction systems, and consider both periodic or random statistically homogeneous ergodic cases. We also consider a diluted Bernoulli percolation model. The homogenization and Γ-convergence approach will be used.

This is a joint work with A. Braides (Roma)

**J.M. Sanz-Serna** (UVA)

*Hybrid Monte-Carlo on Hilbert spaces*

The Hybrid Monte-Carlo (HMC) algorithm provides a framework for sampling from complex, high-dimensional target distributions. In contrast with standard Markov-chain Monte Carlo (MCMC) algorithms, it generates non-local, non-symmetric moves in the state space, alleviating random-walk type behaviour for the simulated trajectories. However, similarly to algorithms based on random walk or Langevin proposals, the number of steps required to explore the target distribution typically grows with the dimension of the state space. We define a generalized HMC algorithm which overcomes this problem for target measures arising as finite-dimensional approximations to measures π which have a density with respect to a Gaussian measure on an infinite-dimensional Hilbert space. The key is to construct an MCMC method which is well defined on the Hilbert space itself. We successively address the following issues in the infinite-dimensional setting of a Hilbert space: (i) construction of a probability measure Π in an enlarged phase space having the target π as a marginal, together with a Hamiltonian flow that preserves Π; (ii) development of a suitable geometric numerical integrator for the Hamiltonian flow; and (iii) derivation of an accept reject/rule to ensure preservation of Π when using the above numerical integrator instead of the actual Hamiltonian flow.

**Nadia Sidorova** (UCL)

*A conditioning principle for Galton-Watson trees*

We discuss the behaviour of a Galton-Watson tree conditioned on its martingale limit being small. We prove that it converges to the smallest possible tree, giving an example of entropic repulsion where the limit has no entropy. We also discuss the first branching time of the conditioned tree (which turns out to be almost deterministic) and the strength of the first branching.
Joint work with N.Berestycki (Cambridge), N.Gantert (Munich), P.Moerters (Bath).

**Konstantinos Spiliopoulos** (Brown University)

*Large deviations and Monte Carlo methods for multiscale diffusions and energy landscapes*

We discuss the large deviations principle and the problem of designing asymptotically optimal importance sampling schemes for stochastic differential equations with small noise and fast oscillating coefficients. There are three possible regimes depending on how fast the intensity of the noise goes to zero relative to the homogenization parameter. We use weak convergence methods which provide us with convenient representations for the action functional for all three regimes. The situation changes completely depending on the regime. Furthermore, we derive a control that nearly achieves the large deviations lower bound at the prelimit level. This control is useful for designing efficient importance sampling schemes for the estimation of rare event probabilities. Standard Monte Carlo methods perform poorly in these kind of problems in the small noise limit. Apart from the smallness of the noise, an additional reason for this is the presence of the fast oscillating coefficients. The construction of the optimal change of measure is based on subsolutions

for an associated Hamilton-Jacobi-Bellman (HJB) equation. These results have applications in chemical physics and biology, where the space is high dimensional. Examples and simulation results will be provided.

**Gabriel Stoltz** (CERMICS)

*Nonequilibrium shear viscosity computations with Langevin dynamics*
(in collaboration with Remi Joubaud)

We study the mathematical properties of a nonequilibrium Langevin dynamics which can be used to estimate the shear viscosity of a system. More precisely, we prove a linear response result which allows to relate averages over the nonequilibrium stationary state of the system to equilibrium canonical expectations. We then write a local conservation law for the average longitudinal velocity of the fluid, and show how, under some closure approximation, the viscosity can be extracted from this profile. We finally characterize the asymptotic behavior of the velocity profile, in the limit where either the transverse or the longitudinal friction go to infinity. Some numerical illustrations of the theoretical results are also presented.

**Tim Sullivan** (California Institute of Technology)

*Optimal uncertainty quantification*

Uncertainty Quantification (UQ) entails understanding how information (or uncertainty) propagates through systems to produce information (or uncertainty) about output quantities of interest. In many applications, this information propagation spans multiple components or scales. In the Optimal UQ (OUQ) framework, these problems are formalized as the study of optimization problems over infinite-dimensional spaces of probability measures and transfer functions.

This talk will cover the fundamental results of the OUQ approach, in particular the Markov—Krein-like theorems that reduce these infinite-dimensional optimization problems to equivalent finite-dimensional ones. Several examples and applications will be illustrated, including optimal concentration-of-measure inequalities, applications to PDEs with multiple scales, optimal bounds on functionals of partially-observed Lipschitz functions, and high-dimensional seismic safety examples.

Joint work with M. McKerns (Caltech/NIST), D. Meyer (T.U. Munich), M. Ortiz (Caltech), H. Owhadi (Caltech), C. Scovel (Los Alamos Nat. Lab.) and F. Theil (Warwick).

**Eric Vanden-Eijnden** (Courant)

*Dimension reduction, coarse-graining and data assimilation in high-dimensional dynamical systems: modeling and computational issues*

Modern computing technologies, such as massively parallel simulation, special-purpose high-performance computers, and high-performance GPUs permit to simulate complex high-dimensional dynamical systems and generate time-series in amounts too large to be grasped by traditional "look and see" analyses. This calls for robust and automated methods to extract the essential structural and dynamical properties from these data in a manner that is little or not depending on human subjectivity. To this end, a decade of work has led to the development of analysis techniques which rely on the partitioning of the conformation space into discrete substates and reduce the dynamics to transitions between these states. A particular successful class of methods of this type are Markov state models (MSMs), in which the transitions between the states in the partition are assumed to be memoryless jumps. The accuracy of these models crucially depends on the choice of these states. In this talk, I will discuss systematic strategies that permit to identify these states and quantify the error of the resulting approximation. These methods will be illustrated on examples arising from molecular dynamics simulations of biomolecules.

**Jonathan Weare** (Chicago)

*Some coarse graining results in crystal surface relaxation*

I will present resent results on the coarse graining of two models of crystal surface relaxation. First I discuss joint work with Hala Al Hajj Shehadeh and Robert V. Kohn on an ODE model of a 1D monotone crystal surface. We prove that the slope of a fnite size crystal in this setting converges (in the long time limit) to a similarity solution. We also give an informal derivation of a fully non-linear fourth order PDE (large crystal) limit of the ODE's as well as analogues of our similarity results in the continuum. Next I'll discuss current work with Jeremy Marzuola investigating certain scaling limits of a general family of Kinetic Monte Carlo models of crystal surface relaxation. We informally derive two fully non-linear fourth order PDE in two different scaling limits. Both PDE's are similar to (but not exactly the same as) PDE's that have been proposed as large scale limits for the models in question. Our aim is to clarify how each arrises as well as to establish the limits rigorously.

**Maria Westdickenberg** (Georgia Institute of Technology)

*Invariant measure of the Allen-Cahn equation: the regime of small temperature and large system size*

It is well-known that for fixed system size and temperature decreasing to zero, the invariant measure of the stochastically perturbed Allen-Cahn equation concentrates on minimizers of the associated (deterministic) energy functional. Roughly speaking, the likelihood to stray significantly from one of these minimizers is exponentially unlikely, with an exponential factor that comes from the energy. When the system size is allowed to grow significantly with decreasing temperature, a new entropic effect enters the picture. We explore the entropic effect for systems that grow up to exponentially with respect to the inverse noise strength. Our methods include reflection arguments, energetic insight, and breaking up the large system into subsystems of a different scale.

**Johannes Zimmer** (Bath)

*The Jacobi-Maupertuis formulation of Hamiltonian dynamics: applications as string method and in homogenisation*

The principle of formulating Hamiltonian trajectories as a geodesic problem is a classic one; we show here that this formulation offers some advantages: (i) the existence of long-time solutions to the Hamiltonian boundary value problem can be shown in a constructive way; this approach gives rise to a convergence proof for an associated string method. (ii) The homogenisation of Hamiltonian dynamics via this principle offers an alternative to the homogenisation via Hamilton-Jacobi theory. We discuss these two approaches for a one-dimensional model problem and present a framework for homogenisation via the Jacobi-Maupertuis approach in several space dimensions.
This is joint work with Hartmut Schwetlick and Daniel Sutton (Bath).