Banff International Research Station
for Mathematical Innovation and Discovery

Numerical Analysis of Multiscale Computations
December 6-11, 2009

MEALS

*Breakfast (Buffet): 7:00 – 9:30 am, Sally Borden Building, Monday – Friday
*Lunch (Buffet): 11:30 am – 1:30 pm, Sally Borden Building, Monday – Friday
*Dinner (Buffet): 5:30 – 7:30 pm, Sally Borden Building, Sunday – Thursday
Coffee Breaks: As per daily schedule, 2nd floor lounge, Corbett Hall
***Please remember to scan your meal card at the host/hostess station in the dining room for each meal.**

MEETING ROOMS

All lectures will be held in Max Bell 159 (Max Bell Building accessible by walkway on 2nd floor of Corbett Hall). LCD projector, overhead projectors and blackboards are available for presentations. *Please note that the meeting space designated for BIRS is the lower level of Max Bell, Rooms 155-159. Please respect that all other space has been contracted to other Banff Centre guests, including any Food and Beverages in those areas.*

SCHEDULE

Sunday

16:00 Check-in begins (Front Desk – Professional Development Centre - open 24 hours)

17:30-19:30 Buffet Dinner

20:00 Informal gathering in 2nd floor lounge, Corbett Hall
Beverages and small assortment of snacks available on a cash honour-system.

Monday

7:00-8:45 Breakfast

8:45-9:00 Introduction and Welcome to BIRS by BIRS Station Manager, Max Bell 159

9:00-9:45 **Rafael Delgado-Buscalioni**, *Tools for multiscale simulations of molecular liquids*

9:45-10:15 Coffee Break, 2nd floor lounge, Corbett Hall

10:15-11:00 **Mitch Luskin**, *Predictive and Efficient Quasicontinuum Methods*

11:00-11:45 **Antoine Gloria**, *Reduction of the resonance error in numerical homogenization*

11:45-13:00 Lunch

13:00-14:00 Guided Tour of The Banff Centre; meet in the 2nd floor lounge, Corbett Hall

14:00-14:45 **Assyr Abdulle**, *Adaptive finite element heterogeneous multiscale methods*

14:45-15:15 Coffee Break, 2nd floor lounge, Corbett Hall

15:15-16:00 **Tony Lelièvre,** *Effective dynamics for the overdamped Langevin equation*

16:15-17:00 **Aleksandar Donev,** *A Hybrid Particle-Continuum Method for Hydrodynamics of Complex Fluids*

17:15-18:00 **Evangelia Kalligiannaki,** *TBA*

18:00-19:30 Dinner

Tuesday

7:00-9:00 Breakfast

9:00-9:45 **Luigi Delle Site,** *Coupling different levels of resolution in molecular simulations*

9:45-10:15 Coffee Break, 2nd floor lounge, Corbett Hall

10:15-11:00 **J M Sanz-Serna,** *The method of averaging, formal series and numerical integrators*

11:00-11:45 **Eric Cances,** *The microscopic origin of the dielectric permittivity of materials*

11:45-13:15 Lunch

13:15-14:00 **Leonid Beryland,** *Homogenization approximation in problems with non-separated scales via a transfer property of the flux norm*

14:00-14:15 Group Photo (meet on the front steps of Corbett Hall)

14:15-15:00 **Shi Jin,** *A class of asymptotic preserving schemes for kinetic equations and related problems with stiff sources*

15:00-15:30 Coffee Break, 2nd floor lounge, Corbett Hall

15:30-16:15 **Nick Tanushev,** *Interaction of scales in ray based methods for wave propagation*

16:15-17:00 **Uri Ascher,** *Point cloud consolidation and surface mesh reconstruction*

17:00-19:30 Dinner

Wednesday

7:00-9:00 Breakfast

9:00-9:45 **Eric Darve,** *Symplectic integrators with adaptive time stepping*

10:00-10:45 **Gunnar Martinsson,** *Fast and accurate techniques for computing Schur complements and performing numerical coarse graining*

11:30-13:30 Lunch

Free Afternoon

17:30-19:30 Dinner

Thursday

7:00-9:00 Breakfast

9:00-9:45 **Claude Le Bris,** *Some numerical approaches for stochastic homogenization*

9:45-10:15 Coffee Break, 2nd floor lounge, Corbett Hall

10:15-11:00 **Valery Smyshlyaev,** *Higher-order and high-contrast homogenization: analytical aspects and applications to dispersion and localization of waves*

11:00-11:45 **Houman Owhadi,** *Non-intrusive and structure preserving multiscale integration of stiff ODEs, SDEs, Hamiltonian systems and Langevin equations with hidden slow dynamics via flow averaging*

11:45-13:30 Lunch

13:30-14:15 **Nawaf Bou-Rabee,** *Solving SDEs using Monte Carlo*

14:15-15:00 **Lexing Ying,** *Recent progress on fast algorithms for electron structure calculation*

15:00-15:30 Coffee Break, 2nd floor lounge, Corbett Hall

15:30-16:15 **Serge Prudhomme,** *Adaptive Modeling based on Optimal Control for Atomistic-to-Continuum Coupled Simulations*

17:30-19:30 Dinner

Friday

7:00-9:00 Breakfast

9:00- Informal Discussions

10:00-11:00 Coffee Break, 2nd floor lounge, Corbett Hall

11:30-13:30 Lunch

Checkout by 12 noon.

You are welcome to use the BIRS facilities (2nd Floor Lounge, Max Bell Meeting Rooms, Reading Room) until 3 pm on Friday, although participants are still required to checkout of the guest rooms by 12 noon.

Banff International Research Station
for Mathematical Innovation and Discovery

Numerical Analysis of Multiscale Computations
December 6-11, 2009

ABSTRACTS

Assyr Abdulle (Ecole Polytechnique Fédérale de Lausanne)

Title: *Adaptive finite element heterogeneous multiscale methods*

Abstract: In this talk we discuss some recent results on adaptive techniques for the finite element heterogeneous multiscale method and present a general framework to derive explicit residual based upper and lower a posteriori bounds on the error. Numerical experiments on various problems will be discussed.

Uri Ascher (University of British Columbia)

Title: Point cloud consolidation and surface mesh reconstruction

Leonid Beryland (Penn State University)

Title: *Homogenization approximation in problems with non-separated scales via a transfer property of the flux norm*

Abstract: In a joint work with H. Owhadi (Caltech), we consider divergence-form scalar elliptic equations and vectorial equations for elasticity with rough ($L^\infty(\Omega)$, $\Omega \subset R^d$) coefficients $a(x)$ that, in particular, model media with non-separated scales and high contrast in their material properties. While the homogenization of PDEs with periodic or ergodic coefficients and well separated scales is now well understood, we consider here the most general case of arbitrary bounded coefficients. For such problems (both scalar divergence form and elasticity) we establish two finite dimensional approximations of solutions, which we refer to as homogenization approximations:

- an approximation by a global basis with an explicit and optimal error constant independent of the contrast and regularity of the coefficients.
- an approximation with a minimal amount of pre-computation with both global and local bases.

We define the flux norm, which is equivalent to the usual H^1-norm, as the L^2 norm of the potential part of the fluxes of solutions. We show that in this norm, the error associated with approximating (in a properly defined finite-dimensional space) the solution to the aforementioned PDE with rough coefficients is equal to the error associated with approximating the solution to the same type of PDE with smooth coefficients in a standard space (e.g., piecewise polynomial). We refer to this property as the transfer property. The results mentioned above are obtained as an application of the transfer property as well as a new class of elliptic inequalities, which play the same role in our approach as the div-curl lemma in classical homogenization

Eric Cances (ENPC and INRIA)

Title: *The microscopic origin of the dielectric permittivity of materials*

Abstract: Several multiscale models coupling an atomistic description of matter on the one hand, and a continuum description on the other hand, have been proposed in the past decades. Such models are widely used in chemistry and molecular biology (continuum solvation models of Poisson-Boltzmann type) as well as in materials science (e.g. quasi-continuum models). However, the theoretical foundations of these models and of the coupling between atomistic and continuum regions are still largely unexplored, and are often a matter of debate. In this talk, I will focus on the specific difficulty originating from the long-range character of the Coulomb potential. I will explain in detail the link between the slow decay of the Coulomb potential and the dielectric permittivity of crystalline materials and argue that atomistic/continuum multiscale models should properly take into account this long-range effect.

Eric Darve (Stanford University)

Title: *Symplectic integrators with adaptive time stepping*

Abstract: Symplectic integrators have several desirable properties for molecular dynamics simulations such as their long time scale energy conservation. Traditional symplectic integrators such as Velocity Verlet use a fixed time step. This may lead to difficulties in particular when dealing with singular force fields such as $1/r$ for Coulombic forces and $1/r^{12}$ for the Lennard-Jones core potential. For these potentials, a fixed time step may lead to spurious energy drift or jump each time two particles get close to each other, because the time step is not able to resolve this "collision" accurately. We will present a new framework that allows in effect adjusting the time step in order to resolve such singularities in the potential. The stability of the method is guaranteed even for thermally equilibrated systems (for example using a Langevin or Brownian formulation), for which the kinetic energy may become arbitrarily large and the collisions arbitrarily stiff. More generally, the framework allows using different time steps for a given term in the potential energy, so that the computational cost, at a given accuracy, can be reduced.

Rafael Delgado-Buscalioni (Autonomous University of Madrid)

Title: *Tools for multiscale simulations of molecular liquids*

Abstract: The art of multiscale simulations have flourished during this decade. Many different approaches to this (wide) problem have been proposed so far but frequently, each method has been designed to tackle a different, particular scenario. This workshop gives a good opportuinity to start connecting different methodologies in the search for a broader panorama. From the standpoint of mathematics, a group of authors have been working on "general theoretical frameworks" for multiscale simulation which may bridge time and space scales and avoid prior knowledge of macroscopic constitutive relations [see for instance, arXiv:Physics/0209043v1]. However, when applying any theoretical multiscale framework to molecular liquids one soon finds great difficulties or bottlenecks associated to practical endeavours, such as how to "lift" (or construct from scratch) a statistically meaningful microscopic configuration or how to impose a macroscopic (or coarse-grained) state at the boundaries of a open molecular simulation. In the first part of the talk I will present several methods (some of them mature enough) which may become standard tools for more general methodologies, such like patch dynamics [for a general review, see Computing in Science and Engineering, 7, 47, 2005]. I will focus on multiscale modelling of liquids ranging from classical

molecular dynamics to continuum hydrodynamics. So far we have been using these tools in (bottom-up) hybrid simulations based on domain decomposition [Phys. Rev. E 76, 036709 (2007)]. The hardest part of the continuum and molecular hydrodynamics coupling is to impose the external thermodynamic and hydrodynamic state into the microscopic simulation. Note that this task is ubiquitous when dealing with two-way coupling and, in particular, it is also present in patch or gaptooth dynamics. We designed a technique (openMD) [Phys. Rev. E 72, 026703 (2005)] to impose external momentum and energy fluxes as boundary conditions to open molecular systems. Local thermo- and hydrodynamics are controlled by the mechanical and thermal energy input into the molecular box. For instance, one can sample the grand canonical ensemble or other processes evolving at a certain (external) condition, like constant enthalpy, constant heat or momentum flux, etc. A great problem in open molecular simulations is how to insert large molecules into an atomistic system. We are solving this problem [J. Chem. Phys. 128, 114110 (2008)] via the Adaptive Resolution Scheme (AdResS) which allows for a gradual switching on/off of the fast degrees of freedom of the entering/ leaving molecules. AdResS is being used in other related scenarios and its full potential is still being explored. During the second part of the talk I would like to present some new research on coarse or effective models which involve a large reduction of degrees of freedom in molecular systems. In particular, I'll mention a recent work [Faraday Discuss., 144, 301 (2010)] on coarse-graining of large molecules (star polymers) which presents an operational route to evaluate the different terms (effective potential, friction and noise) needed to properly describe the dynamics of coarse-grained variables (molecule's center of mass). Finally, I'll try to illustrate the minimum model capable to describe the essential dynamics of a polymer under shear flow, solved via a 1D Fokker-Planck equation. Not only the success but also the failures of these effective models might provide important information about the system.

Luigi Delle Site (Max-Planck Institut für Polymerforschung)

Title: *Coupling different levels of resolution in molecular simulations*

Abstract:

Simulation schemes that allow to change molecular representation in a subvolume of the simulation box while preserving the equilibrium with the surrounding introduce conceptual problems of thermodynamic consistency. In this talk I present a general scheme based on thermodynamic arguments which ensures thermodynamic equilibrium among the molecules of different representation. The robustness of the algorithm is tested for two examples, namely an adaptive resolution simulation, atomistic/coarse-grained, for a liquid of tetrahedral molecules and an adaptive resolution simulation of a binary mixture of tetrahedral molecules and spherical solutes. Also the extension of the method to the description of some basic quantum effects will be discussed.

Aleksandar Donev (Lawrence Berkeley National Laboratory)

Title: *A Hybrid Particle-Continuum Method for Hydrodynamics of Complex Fluids*

Abstract: We generalize a previously-developed hybrid particle-continuum method [J. B. Bell, A. Garcia and S. A. Williams, SIAM Multiscale Modeling and Simulation, 6:1256-1280, 2008] to dense fluids and two and three dimensional flows. The scheme couples an explicit fluctuating compressible Navier-Stokes solver with the Isotropic Direct Simulation Monte Carlo (DSMC) particle method [A. Donev and A. L. Garcia and B. J. Alder, ArXiv preprint 0908.0510]. To achieve bidirectional dynamic coupling between the particle (microscale) and continuum (macroscale) regions, the continuum solver provides state-based boundary conditions to the particle domain, while the particle domain provides

flux-based boundary conditions for the continuum solver, thus ensuring both state and flux continuity across the particle-continuum interface. A small mismatch is observed between the mean density and temperature in the particle and continuum regions that comes from the finite size of the hydrodynamic cells used to estimate mean hydrodynamic values. By calculating the dynamic structure factor for both a 'bulk' (periodic) and a finite system, we verify that the hybrid algorithm is capable of accurately capturing the propagation of spontaneous thermal fluctuations across the particle-continuum interface. We then study the equilibrium diffusive motion of a large spherical bead suspended in a particle solvent and find that the hybrid method correctly reproduces the velocity autocorrelation function of the bead only if thermal fluctuations are included in the continuum solver. Finally, we apply the hybrid to the well-known adiabatic piston problem and find that the hybrid correctly reproduces the slow non-equilibrium relaxation of the piston toward thermodynamic equilibrium when fluctuations are included in the continuum solver. These examples clearly demonstrate the need to include fluctuations in continuum solvers employed in hybrid multiscale methods.

Antoine Gloria (INRIA Lille – Nord Europe)

Title: *Reduction of the resonance error in numerical homogenization*

Abstract: This talk is concerned with the approximation of effective coefficients for the homogenization of linear elliptic equations, and more generally with numerical homogenization. One common drawback among numerical homogenization methods is the presence of the so-called resonance error, which roughly speaking is a function of the ratio H/ε, where H is a typical macroscopic lengthscale and ε is the typical size of the heterogeneities. We propose an alternative for the computation of homogenized coefficients and correctors, and prove that the formulation is asymptotically consistent within the homogenization framework. We also give a complete error analysis in the locally periodic case and in a stochastic case, which show the interest of the approach in terms of reduction of the resonance error. Numerical tests confirm the sharpness of the estimates. We will conclude the talk by showing how to combine this approach with standard numerical homogenization methods.

Shi Jin (University of Wisconsin, Madison)

Title: *A class of asymptotic preserving schemes for kinetic equations and related problems with stiff sources*

Abstract: we propose a general time discrete framework to design asymptotic preserving schemes for the Boltzmann kinetic and related equations. Numerically solving these equations are challenging due to the nonlinear stiff collision (source) terms induced by small mean free or relaxation time. We propose to penalize the nonlinear collision term by a BGK-type relaxation term, which can be solved explicitly even if discretized implicitly in time. Moreover, the BGK-type relaxation operator helps to drive the density distribution toward the local Maxwellian, thus naturally imposes an asymptotic-preserving scheme in the Euler limit. The scheme so designed does not need any nonlinear iterative solver or the use of Wild Sum. It is uniformly stable in terms of the (possibly small) Knudsen number, and can capture the macroscopic fluid dynamic (Euler) limit even if the small scale determined by the Knudsen number is not numerically resolved. It is also consistent to the compressible Navier-Stokes equations if the viscosity and heat conductivity are numerically resolved. The method is applicable to many other related problems, such as hyperbolic systems with stiff relaxation, and high order parabolic equations.

Evangelia Kalligiannaki (University of Tennessee and Oak Ridge National Laboratory)

Title: *TBA*

Claude Le Bris (CERMICS ENPC)

Title: *Some numerical approaches for stochastic homogenization*

Abstract: The talk will overview some recent results obtained in collaboration with X. Blanc (CEA), A. Anantharaman, R. Costaouec and F. Legoll (Ecole des Ponts) on new numerical approaches for homogenization problems that involve 'some' randomness. In particular, the case of periodic media weakly modified by random perturbations will be examined. Some preliminary results will also be presented, that show that techniques for reducing the variance in fully stochastic problems can be successfully implemented.

Tony Lelièvre (ENPC)

Title: *Effective dynamics for the overdamped Langevin equation*

Abstract: We consider a system described by a high-dimensional variable X_t that evolves according to the overdamped Langevin equation, and a scalar function $\xi(X)$ of the state variable X, representing a coarse-grained information. We propose an effective closed dynamics that approximates the evolution of $\xi(X_t)$. The accuracy of this effective dynamics compared to the original one is analyzed through error estimates between the marginals in time of the two processes. Numerical simulations illustrate the efficiency of the approach as well as the accuracy of the proposed dynamics according to various criteria, including residence times in potential energy wells. This is a joint work with Frédéric Legoll, see `http://fr.arxiv.org/abs/0906.4865`

Xiantao Li (Penn State University)

Title: *Multiscale simulations of the dynamics of solids*

Abstract: We discuss a multiscale method to simulate dynamics of defects in crystalline solids. The idea is based on the heterogeneous multiscale method, and we will mainly focus on the coupling conditions. As an example, we simulate a brittle crack in Iron under various types of loading conditions.

Mitch Luskin (University of Minnesota)

Title: *Predictive and Efficient Quasicontinuum Methods*

Abstract: The formation and motion of lattice defects such as cracks, dislocations, or grain boundaries, occurs when the lattice configuration loses stability, that is, when an eigenvalue of the Hessian of the lattice energy functional becomes negative. When the atomistic energy is approximated by a hybrid energy that couples atomistic and continuum models, the accuracy of the approximation can only be guaranteed near deformations where both the atomistic energy as well as the hybrid energy are stable. We propose, therefore, that it is essential for the evaluation of the predictive capability of atomistic-to-continuum coupling methods near instabilities that a theoretical analysis be performed, at least for some representative model problems, that determines whether the hybrid energies remain stableup

to the onset of instability of the atomistic energy. In joint work with Matthew Dobson and Christoph Ortner, we formulate a one-dimensional model problem with nearest and next-nearest neighbor interactions and use rigorous analysis, asymptotic methods, and numerical experiments to obtain such sharp stability estimates for the basic quasicontinuum approximations and to distinguish which methods reproduce the stability of the atomistic system.

Gunnar Martinsson (University of Colorado at Boulder)

Title: *TBA*

Houman Owhadi (California Institute of Technology)

Title: *Non-intrusive and structure preserving multiscale integration of stiff ODEs, SDEs, Hamiltonian systems and Langevin equations with hidden slow dynamics via flow averaging*

Abstract: We present a new class of integrators for stiff ODEs as well as SDEs. An example of subclass of systems that we treat are ODEs and SDEs that are sums of two terms one of which has large coefficients. These integrators are (i) *Multiscale:* they are based on flow averaging and so do not resolve the fast variables but rather employ step-sizes determined by slow variables (ii) *Basis:* the method is based on averaging the flow of the given dynamical system (which may have hidden slow and fast processes) instead of averaging the instantaneous drift of assumed separated slow and fast processes. This bypasses the need for identifying explicitly (or numerically) the slow or fast variables. (iii) *Non intrusive:* A pre-existing numerical scheme resolving the microscopic time scale can be used as a black box and turned into one of the integrators in this paper by simply turning the large coefficients on over a microscopic timescale and off during a mesoscopic timescale. (iv) *Convergent over two scales:* strongly over slow processes and in the sense of measures over fast ones. We introduce the related notion of two scale flow convergence and analyze the convergence of these integrators under the induced topology. (v) *Structure preserving:* For stiff Hamiltonian systems (possibly on manifolds), they are symplectic, time-reversible, and symmetric (under the group action leaving the Hamiltonian invariant) in all variables. They are explicit and apply to arbitrary stiff potentials (that need not be quadratic). Their application to the Fermi-Pasta-Ulam problems shows accuracy and stability over 4 orders of magnitude of time scales. For stiff Langevin equations, they are symmetric (under a group action), time-reversible and Boltzmann-Gibbs reversible, quasi-symplectic on all variables and conformally symplectic with isotropic friction. This is a joint work with Molei Tao and Jerry Marsden.

Serge Prudhomme (The University of Texas at Austin)

Title: *Adaptive Modeling based on Optimal Control for Atomistic-to-Continuum Coupled Simulations*

Abstract: The development of multiscale approaches for nanoscale simulations has become an important research area that aims at combining concurrent models in order to capture the different scales observed in complex problems. The main idea is to replace a reference particle model, supposedly intractable, by a coupled model that blends solutions from small and large scale models. In this work, a continuum (large scale) model is used far from the regions of interest and a particle (small scale) model is kept in the local critical regions; the two models are then coupled together based on the Arlequin framework. It is important to observe that such a multiscale model only constitutes a surrogate model of the initial particle model. Errors arising from the approximation by this surrogate model must therefore be estimated and controlled. We will present an adaptive method based on

optimal control in which modeling errors are controlled with respect to specific quantities of interest. We will present recent results for one- and two-dimensional problems.

J M Sanz-Serna (Universidad de Valladolid)

Title: *The method of averaging, formal series and numerical integrators*

Abstract: B-series and related series are a common tool in the analysis of numerical methods for ODEs. In the talk I will discuss (i) the use of B-series within the analytic method of averaging and (ii) the use of B-series in the analysis of numerical time-steppers based on the multiscale approach.

Valery Smyshlyaev (University of Bath)

Title: *Higher-order and high-contrast homogenization: analytical aspects and applications to dispersion and localization of waves*

Abstract: "Classical" homogenization derives homogenized equations with homogeneous (or slowly varying) coefficients from the same class as the original ones, with rapidly varying coefficients. It is therefore intrinsically incapable of accounting for such effects as, for example, dispersion and localization due to the micro-macro interaction (in particular to "micro-resonances"). We review recent advances in "higher-order" homogenization which, combining asymptotic and variational techniques, allows to rigorously derive higher-order homogenized equations which on one hand do account for such effects and on the other hand provided higher-order error bounds in an appropriate sense. The role of the higher-order effects increases with the contrast, and for a critically scaled contrast the limit asymptotic descriptions remain multiscale ones although often (more) explicit. This leads to the interesting effects physically, and mathematically requires developing novel versions of e.g. multiscale convergence and of the theory of compensated compactness, and is hoped to stimulate novel numerical approaches.

Nick Tanushev (The University of Texas at Austin)

Title: *Interaction of scales in ray based methods for wave propagation*

Abstract: We will briefly introduce asymptotic ray based methods for high frequency wave propagation with an emphasis on Gaussian beams. We will discuss challenges that occur when variations in the sound speed interact with the small scale oscillations of the waves, computational methods for overcoming these difficulties and, finally, some open problems.

Eric Vanden-Eijnden (New York University)

Title: *A general strategy for the design of seamless multiscale methods*

Abstract: I will present a new general framework for designing multiscale methods. Compared with previous work such as Brandt's systematic up-scaling, the heterogeneous multiscale method and the "equation-free" approach, this new framework has the distinct feature that it does not require reinitializing the microscale model at each macro time step or each macro iteration step. In the new strategy, the macro- and micro-models evolve simultaneously using different time steps (and therefore different clocks), and they exchange data at every step. The micro-model uses its own appropriate time step. The macro-model runs at a slower pace than required by accuracy and stability considerations for the macroscale dynamics, in order for the micro-model to relax. I will discuss the

relation of new seamless method with techniques such as HMM, and present applications to a toy system used in climatic studies, to the modeling of complex fluids, and to free energy calculations in molecular dynamics.

This is joint work with Weinan E and Weiqing Ren with applications performed in collaboration with Ibrahim Fatkullin and Luca Maragliano.

Lexing Ying (The University of Texas at Austin)

Title: *Recent progress on fast algorithms for electron structure calculation*