Workshop on Mathematical Theory and Computational Methods for Multiscale Problems
(9 - 13 Jan 2012)

Venue: IMS Auditorium
Institute for Mathematical Sciences, NUS
3 Prince George's Park, Singapore 118402
Tel: 6516 1897

Monday, 9 Jan 2012	
08:45am - 09:00am	Registration
09:00am - 09:10am	Opening Remarks *Louis Chen, Institute for Mathematical Sciences* *Member of the Local Organizing Committee*
	Chair: Weizhu Bao, National University of Singapore
09:10am - 10:00am	On the multi-dimensional compressible Navier-stokes *Zhouping Xin, Chinese University of Hong Kong, Hong Kong*
10:00am - 10:30am	*--- Coffee Break ---*
10:30am - 11:20am	Finite element zooms for localized multiscale problems *Olivier Pironneau, University of Paris VI, France*
11:20am - 12:10pm	Stability of rarefaction waves to the 1D compressible Navier-Stokes equations with density-dependent viscosity *Quansen Jiu, Capital Normal University, China*
12:10pm - 02:00pm	*--- Lunch Reception at IMS ---*
	Chair: Zhouping Xin, Chinese University of Hong Kong, Hong Kong
02:00pm - 02:50pm	Some recent mathematical contributions to multiscale modelling for polymeric fluids *Tony Lelievre, École Nationale Des Ponts Et Chaussées, France*
02:50pm - 03:40pm	A seamless multiscale method and its application to complex fluids *Weiqing Ren, Institute for High Performance Computing and National University of Singapore*
03:40pm - 04:20pm	*--- Group Photo & Coffee Break ----*
04:20pm - 05:10pm	Drift-diffusion-recombination processes in excitonic organic photovoltaic devices *Klemens Fellner, University of Cambridge, UK*

Tuesday, 10 Jan 2012	
08:45am - 09:00am	Registration
	Chair: David Srolovitz, Institute for High Performance Computing and National University of Singapore
09:00am - 09:50am	Nonlocal diffusion, nonlocal mechanics, and a nonlocal vector calculus *Max Gunzburger, Florida State University, USA*
09:50am - 10:40am	Atomistic-to-Continuum coupling methods *Mitchell Luskin, University of Minnesota, USA*
10:40am - 11:10am	--- *Coffee Break* ----
11:10am - 12:00nn	Topology and geometry versus atomistics and chemistry of low-dimensional materials *Boris Yakobson, Rice University, USA*
12:00nn - 02:00pm	--- *Lunch* ---
	Chair: Mitchell Luskin, University of Minnesota, USA
02:00pm - 02:50pm	Asymptotic-Preserving schemes for kinetic-fluid modeling of two phase flows *Shi Jin, University of Wisconsin, USA*
02:50pm - 03:40pm	Asymptotic-preserving IMEX schemes for kinetic equations and related hyperbolic problems *Lorenzo Pareschi, University of Ferrara, Italy*
03:40pm - 04:20pm	--- *Coffee Break* ----
04:20pm - 05:10pm	Effective boundary conditions for the Stokes fluid with thin coatings via homogenization *Zhengan Yao, Sun Yat-sen University, China*
06:30pm - 07:30pm	**Public Lecture:** Carbons: From Diamonds to Space Elevator and Future Electronics *Boris Yakobson, Rice University, USA* Venue: LT31, Block S16, Level 3, National University of Singapore Singapore 117543

Wednesday, 11 Jan 2012	
08:40am - 09:00am	Registration
	Chair: Max Gunzburger, Florida State University, USA
09:00am - 09:50am	Optimization-based computational modeling Pavel Bochev, Sandia National Laboratories, USA
09:50am - 10:40am	How to compute transition states/saddle points? *Qiang Du, Penn State University, USA*
10:40am - 11:10am	--- *Coffee Break* ---
11:10am - 12:00nn	Numerical study of phase and phase transition based on nonlinear variation *Pingwen Zhang, Peking University, China*
12:00nn - 02:00pm	--- *Lunch* ---
	Chair: Shi Jin, University of Wisconsin, USA
02:00pm - 02:50pm	Quantum semiconductor devices: analysis and simulation *Ansgar Juengel, Institute for Analysis and Scientific Computing, Austria*
02:50pm - 03:40pm	Numerical schemes based on a boundary matching micro-macro decomposition for kinetic equations *Florian Méhats, Université de Rennes 1, France*
03:40pm - 04:20pm	--- *Coffee Break* ---
04:20pm - 05:10pm	Dynamics of semiclassical wave packet dynamics in (nonlinear) Schroedinger equations with periodic potentials *Christof Sparber, University of Illinois at Chicago, USA*
06:00pm - 08:00pm	Dinner at NUSSU (Volunteer and self-paid)

Thursday, 12 Jan 2012	
08:45am - 09:00am	Registration
	Chair: Pingwen Zhang, Peking University, China
09:00am - 09:50am	Nonlinear one particle NLS: Multi Configuration Time Dependent Hartree Fock *Norbert Mauser, Universität Wien, Austria*
09:50am - 10:40am	Adaptive time integration methods for Gross-Pitaevski equations *Mechthild Thalhammer, University of Innsbruck, Austria*
10:40am - 11:10am	*--- Coffee Break ----*
11:10am - 12:00nn	Multiscale methods and analysis for the nonlinear Klein-Gordon equation in the nonrelativistic limit regime *Weizhu Bao, National University of Singapore*
12:00nn - 02:00pm	*--- Lunch ---*
	Chair: Olivier Pironneau, University of Paris VI, France
02:00pm - 02:50pm	A stochastic particle approximation for measure solutions of the 2D Keller-Segel system *Christian Schmeiser, University of Vienna, Austria*
02:50pm - 03:40pm	Dimension reduction for dipolar Gross-Pitaevskii equation *Yongyong Cai, National University of Singapore*
03:40pm - 04:20pm	*--- Coffee Break ---*
04:20pm - 05:10pm	A micro/macro parareal algorithm for singularly perturbed ordinary differential equations *Frédéric Legoll, École Nationale Des Ponts Et Chaussées, France*
Friday, 13 Jan 2012	
08:45am - 09:00am	Registration
	Chair: Weiqing Ren, Institute for High Performance Computing and National University of Singapore
09:00am - 09:50am	The low-barrier problem in long-time atomistic dynamics *Arthur Voter, Los Alamos National Laboratory, USA*
09:50am - 10:40am	Multiscale methods for elliptic homogenization problems *Xingye Yue, Soochow University, China*
10:40am - 11:10am	*--- Coffee Break ----*
11:10am - 12:00nn	TBA *Xuan Chun Dong, National University of Singapore*
12:00nn - 12:05pm	Closing Remarks

~Abstract~

Multiscale methods and analysis for the nonlinear Klein-Gordon equation in the nonrelativistic limit regime

Weizhu Bao, National University of Singapore

In this talk, I will review our recent works on numerical methods and analysis for solving the nonlinear Klein-Gordon (KG) equation in the nonrelativistic limit regime, involving a small dimensionless parameter which is inversely proportional to the speed of light. In this regime, the solution is highly oscillating in time and the energy becomes unbounded, which bring significant difficulty in analysis and heavy burden in numerical computation. We begin with four frequently used finite difference time domain (FDTD) methods and obtain their rigorous error estimates in the nonrelativistic limit regime by paying particularly attention to how error bounds depend explicitly on mesh size and time step as well as the small parameter. The we consider a numerical method by using spectral method for spatial derivatives combined with an exponential wave integrator (EWI) in the Gautschi-type for temporal derivatives to discretize the KG equation. Rigorious error estimates show that the EWI spectral method show much better temporal resolution than the FDTD methods for the KG equation in the nonrelativistic limit regime. In order to design a multiscale method for the KG equation, we establish error estimates of FDTD and EWI spectral methods for the nonlinear Schrodinger equation perturbed with a wave operator. Finally, a multiscale method is presented for discretizing the nonlinear KG equation in the nonrelativistic limit regime based on large-small amplitude wave decompostion. This multiscale method converges uniformly in spatial/temporal discretization with respect to the small parameter for the nonlinear KG equation in the nonrelativistic limite regime. Finally, applications to several high oscillatory dispersive partial differential equations will be discussed.

Optimization-based computational modeling

Pavel Bochev, Sandia National Laboratories, USA

We present a new, optimization-based strategy for modeling and simulation of complex multiphysics problems whose constituent components are governed by physical laws with disparate mathematical structures. Our approach relies on optimization and control ideas to (i) assemble and decompose multiphysics operators in a way that enables parallelism, and (ii) preserve their fundamental physical properties in the discretization process. In so doing we are able to synthesize

-> compatible, feature-preserving discretizations of multiphysics problems, from high-resolution compatible discretizations of their constituent physics components, and

-> efficient, scalable multiphysics solvers from fast solvers for their constituent physics components.

The optimization-based modeling and simulation framework departs substantially from the dominnant computational strategies for multiphysics problems. Established approaches treat discretization and solution as

separate tasks, and the former is burdened with the preservation of physical properties such as maximum principles, positivity, or monotonicity. Because our framework assembles discrete multiphysics models from high-resolution discretizations of their constituent physics components, the operator decomposition required for fast, scalable solvers is embedded in the problem formulation from the onset. Our approach also relieves discretization from tasks that impose severe geometric constraints on the mesh, or tangle accuracy and resolution with the preservation of physical properties. Two examples will illustrate the scope of our approach approach: an optimization-based framework for multi-physics coupling, and an optimization-based algorithm for constrained interpolation and transport. This is joint work with D. Ridzal, (Sandia).

Dimension reduction for dipolar Gross-Pitaevskii equation
Yongyong Cai, National University of Singapore

Bose-Einstein condensate (BEC) with dipole-dipole interaction has received considerable research interests recently. At zero temperature, the dipolar BEC is well-described by a three dimensional (3D) Gross-Pitaevskii equation (GPE) with a nonlocal dipole-dipole interaction term. With strongly anisotropic confining potentials, the three dimensional dipolar GPE will result in effective two-dimensional (2D) equation for disk-shaped BEC or effective one-dimensional (1D) equation for cigar-shaped BEC . Upon a new formulation of the 3D dipolar GPE, we obtain the corresponding effective lower dimensional equations. Ground state and dynamics for the 3D and lower dimensional equations are discussed. Extensions to multi-layered dipolar condensate will be also discussed.

How to compute transition states/saddle points?
Qiang Du, Penn State University, USA

Exploring complex energy landscape is a challenging issue in many applications. Besides locating equilibrium states, it is often also important to identify transition states given by saddle points. In this talk, we will discuss existing and new algorithms for the computation of such transition states with a focus on the newly developed Shrinking Dimer Dynamics and present some related mathematical theory on stability and convergence. We will consider a number of applications including the study of frustrations of interacting particles and nucleation in solid state phase transformations.

Drift-diffusion-recombination processes in excitonic organic photovoltaic devices
Klemens Fellner, University of Cambridge, UK

We present some recent results and ongoing work on drift-diffusion-reaction systems modelling organic photovoltaic devices. While classical semiconductors show recombination typically throughout the whole device feature organic photovoltaic devices significant charge generation only in the very proximity of an interface between two different organic polymers. We discuss basic questions of modelling, existence and stationary states. Moreover, we present some interesting asymptotic approximations and discuss the use of entropy.

Joint work with Dan Brinkman, Peter Markowich, Marie-Therese Wolfram (DAMTP, University of Cambridge)

Nonlocal diffusion, nonlocal mechanics, and a nonlocal vector calculus
Max Gunzburger, Florida State University, USA

Based on notions for nonlocal fluxes between volumes and nonlocal balance laws and a nonlocal vector calculus we have developed, we introduce nonlocal models for diffusion and the nonlocal peridynamics continuum model for mechanics. A feature of the nonlocal problems that has important practical consequences are that constraints, e.g., of Dirichlet type, are applied over volumes and not along bounding surfaces. A brief review of the nonlocal calculus is given, including definitions of nonlocal divergence, gradient, and curl operators and derivations of a nonlocal Gauss theorem and Green's identities. Through appropriate limiting processes, relations between the nonlocal operators and their differential counterparts are established.

The nonlocal calculus is used to define weak formulations of the nonlocal diffusion and mechanics problems which are then analyzed, showing, for example, that unlike elliptic partial differential equations, these problems do not necessary result in the smoothing of data. We briefly consider connections to fractional Laplacian problems (which are special cases of our models) and finite element methods for nonlocal problems, focusing on solutions containing jump discontinuities; in this setting, discontinuous Galerkin methods are conforming and nonlocal problems can lead to optimally accurate approximations. We also show how our models can be implemented so that they are multi-scale mono-models, i.e., they are single models that are valid and tractable over a wide range of scales.

Asymptotic-Preserving schemes for kinetic-fluid modeling of two phase flows
Shi Jin, University of Wisconsin, USA

We consider systems coupling the compressible or incompressible Navier-Stokes equations to the Vlasov-Fokker-Planck equation. Such a problem arises in the description of particulate flows. We design numerical schemes to simulate this system. These schemes are asymptotic-preserving, thus efficient in both the kinetic and hydrodynamic regimes. It has a numerical stability condition controlled by the non-stiff convection operator, with an implicit treatment of the stiff drag term and the Fokker-Planck operator. Yet, consistent to a standard asymptotic-preserving Fokker-Planck solver or an incompressible Navier-Stokes solver, only the conjugate-gradient method and fast Poisson and Helmholtz solvers are needed. Numerical experiments are presented to demonstrate the accuracy and asymptotic behavior of the schemes, with several interesting applications.

This is a joint work with T. Goudon, J.-G. Liu and Bokai Yan.

Stability of rarefaction waves to the 1D compressible Navier-Stokes equations with density-dependent viscosity
Quansen Jiu, Capital Normal University, China

In this talk, we will present some recent results on the asymptotic stability of rarefaction waves for the compressible isentropic Navier-Stokes equations with density-dependent viscosity. Thehese results hold for large-amplitudes rarefaction waves and arbitrary initial perturbations. This is joint with Yi Wang and Zhouping Xin.

Quantum semiconductor devices: analysis and simulation
Ansgar Juengel, Institute for Analysis and Scientific Computing, Austria

The microelectronics industry is heavily based on the construction of faster, smaller, and more efficient semiconductor devices. Quantum semiconductor structures might fulfill these requirements also in the future. In this talk, some modeling and simulation approaches for quantum semiconductors will be presented.

First, quantum Navier-Stokes equations will be introduced. This model has a surprising nonlinear structure and posseses two different energy functionals. It is shown how this structure can be used to derive global existence results, and a connection to "Noether symmetries" in a Lagrangian mechanics framework is highlighted.

Second, transient numerical simulations of a 3-D quantum waveguide are presented, based on a time-splitting pseudo-spectral approximation of the Schroedinger equation. Furthermore, self-induced oscillations of a tunneling diode in a small electric circuit are shown.

A micro/macro parareal algorithm for singularly perturbed ordinary differential equations
Frédéric Legoll, École Nationale Des Ponts Et Chaussées, France

We introduce and analyze a micro/macro parareal algorithm for the time-parallel integration of singularly perturbed ordinary differential equations. The system we consider includes some fast and some slow variables, the limiting dynamics of which (in the limit of infinite time scale separation) is known.

The algorithm first computes a cheap but inaccurate macroscopic solution using a coarse propagator (by only evolving the slow variables according to their limiting dynamics). This solution is iteratively corrected by using a fine-scale propagator (simulating the full microscopic dynamics on both slow and fast variables), in the parareal algorithm spirit. The efficiency of the approach will be demonstrated on the basis of numerical analysis arguments and representative numerical experiments.

Joint work with T. Lelievre and G. Samaey.

Some recent mathematical contributions to multiscale modelling for polymeric fluids
Tony Lelievre, École Nationale Des Ponts Et Chaussées, France

In this talk, I will present two recent works concerning multiscale models for polymeric fluids.

First, I will present a numerical closure procedure that we recently proposed in [1] to get, from a microscopic model, a closed macroscopic model. This procedure is related to the so-called quasi-equilibrium approximation method, and can be seen as a justification of this approach.

Second, I will discuss the longtime behaviour of some models for rigid polymers (liquid crystals models). Such models are interesting since their longtime behaviour may be quite complicated, including convergence to periodic in time solutions. I will explain how such convergence can be proven using entropy techniques, see [2].

References:
[1] V. Legat, T. Lelièvre and G. Samaey, A numerical closure approach for kinetic models of polymeric fluids: exploring closure relations for FENE dumbbells, Computers and Fluids, 43, 119-133, (2011).
[2] L. He, C. Le Bris and T. Lelièvre, Periodic long-time behaviour for an approximate model of nematic polymers, http://arxiv.org/abs/1107.3592.

Atomistic-to-Continuum coupling methods
Mitchell Luskin, University of Minnesota, USA

Many materials problems require the accuracy of atomistic modeling in small regions, such as the neighborhood of a cracktip. However, these localized defects typically interact through long-range elastic fields with a much larger region that cannot be computed atomistically. Materials scientists have proposed many methods to compute solutions to these multiscale problems by coupling atomistic models near alocalized defect with continuum models where the deformation isnearly uniform on the atomistic scale. During the past several years, a mathematical structure has been given to the description and formulation of atomistic-to-continuum coupling methods, and corresponding numerical analysis has clarified the relation between the various methods and their sources of error. This lecture will present recent developments for the numerical analysis of atomistic-to-continuum coupling methods.

Nonlinear one particle NLS: Multi Configuration Time Dependent Hartree Fock
Norbert Mauser, Universität Wien, Austria

We show how to obtain "effective one-particle Nonlinear Schrodinger equations" as proximations of the "exact" linear N-particle Schrodinger equations with Coulomb interaction. The simplest "mean field" approximations are "Hartree" equations for boson condensates, like the simple cubic NLS, or Hartree-Fock equations for fermions that contain "exchange interactions" due the Pauli principle.

The Multi Configuration Time Dependent Hartree Fock (MCTDHF) equations are a complicated system of coupled ODEs and PDEs that allows to include "correlation" and that yields an approximation hierarchy that, in principle, converges to the exact model. We present the equations and state-of-the-art mathematical results on local/global well-posedness.

Numerical schemes based on a boundary matching micro-macro decomposition for kinetic equations
Florian Méhats, Université de Rennes 1, France

We introduce a new micro-macro decomposition of collisional kinetic equations in the specific case of the diffusion limit, which naturally incorporates the incoming boundary conditions. The idea is to write the distribution fonction f in all its domain as the sum of an equilibrium adapted to the boundary (which is not the usual equilibrium associated with f) and a remaining kinetic part. This equilibrium is defined such that its incoming velocity moments coincide with the incoming velocity moments of the distribution function. A consequence of this strategy is that no artificial boundary condition is needed in the micro-macro models and the exact boundary condition on f is naturally transposed to the macro part of the model. This method provides an 'Asymptotic preserving' numerical scheme which generates a very good approximation of the space boundary values at the diffusive limit, without any mesh refinement in the boundary layers. Our

numerical results are in very good agreement with the exact so-called Chandrasekhar value, which is known in some simple cases.

Asymptotic-preserving IMEX schemes for kinetic equations and related hyperbolic problems
Lorenzo Pareschi, University of Ferrara, Italy

Implicit-Explicit Runge-Kutta schemes represent a powerful tool for the numerical treatment of stiff terms in partial differential equations. When necessary they can be designed in order to achieve suitable asymptotic preserving (AP) properties of the underlying systems of differential equations, like in the case of hyperbolic systems with relaxation [1]. Recently they have been extended to the case of stiff diffusive limits [2].

Similar techniques can be adopted when dealing with kinetic equation of Boltzmann-type. Here, however, the major challenge is represented by the complicated nonlinear structure of the collisional operator which makes prohibitively expensive the use of fully implicit solvers.
Additional difficulties are given by the need to preserve some relevant physical properties like nonnegativity of the solution and entropy inequality. This problem in the context of splitting methods using exponential techniques has been successfully studied recently in [4].

In this talk, using a penalization approach introduced in [3], we will present some recent advances in this directions and construct IMEX schemes up to third order which are asymptotic preserving for the Boltzmann equation in the fluid-limit without having to invert expensive nonlinear algebraic systems. General conditions on the coefficients of the IMEX schemes in order to satisfy the AP-property are derived and requirements for nonnegativity and entropicity analyzed. Examples of nonnegative and entropic schemes are also discussed. Finally numerical evidence of the effectiveness of the new IMEX schemes for space homogeneous and non homogeneous problems is given. We refer to [5] for further details.

References

[1] L.Pareschi, G.Russo, "Implicit-Explicit Runge-Kutta methods and applications to hyperbolic systems with relaxation", J. Sci. Comp.
(2005)
[2] S.Boscarino, L.Pareschi, G.Russo, "Implicit-Explicit Runge-Kutta schemes for hyperbolic systems and kinetic equations in the diffusion limit", preprint (2011) [3] S. Jin, F. Filbet, "A class of asymptotic-preserving schemes for kinetic equations and related problems with stiff sources", J. Comp.
Phys. (2010)
[4] G. Dimarco, L.Pareschi, "Exponential Runge"Kutta methods for stiff kinetic equations", SIAM J. Num. Anal. (2011) [5] G. Dimarco, L.Pareschi, "Implicit-Explicit Runge-Kutta methods for stiff kinetic equations and related hyperbolic relaxation problems", preprint (2011)

A seamless multiscale method and its application to complex fluids
Weiqing Ren, Institute for High Performance Computing and National University of Singapore

I will present a seamless multiscale method for the study of multiscale problems. The multiscale method aims at capturing the macroscale behavior of the system with the help of a microscale model. The macro model provides the necessary constraint for the micro model and the micro model supplies the missing data (e.g. the constitutive relation or the boundary conditions) for the macro model. In the seamless algorithm, the macro and micro models evolve simultaneously using different time steps, and they exchange data at every step. The micro model uses its own appropriate (micro) time step. The macro model uses a macro time step but runs at a slower pace than required by accuracy and stability considerations in order for the micro dynamics to have sufficient time to adapt to the environment provided by the macro state. The method has the advantage that it does not require the reinitialization of the micro model at each macro time step or each macro iteration step. The data computed from the micro model is implicitly averaged over time. In this talk, I will discuss the algorithm of the multiscale method, the error analysis, and its application to complex fluids.

A stochastic particle approximation for measure solutions of the 2D Keller-Segel system
Christian Schmeiser, University of Vienna, Austria

The 2D parabolic-elliptic Keller-Segel system features finite time concentration effects and global existence of suitably defined measure solutions. A stochastic particle approximation can be used as basis for numerical approximations. Its convergence as the number of particles tends to infinity will be discussed.
This is joint work with Jan Haskovec.

Dynamics of semiclassical wave packet dynamics in (nonlinear) Schroedinger equations with periodic potentials
Christof Sparber, University of Illinois at Chicago, USA

We consider semiclassically scaled Schroedinger equations with an external potential and a highly oscillatory periodic potential. We construct asymptotic solutions in the form of semiclassical wave packets, i.e. coherent states propagating within a given Bloch energy band. These solutions are concentrated (both, in space and in frequency) around the effective semiclassical phase-space flow and involve a slowly varying envelope whose dynamics is governed by a homogenized Schrödinger equation with time-dependent effective mass. In the linear case, the corresponding adiabatic decoupling of the slow and fast degrees of freedom is shown to be valid up to Ehrenfest time scales.

Adaptive time integration methods for Gross-Pitaevski equations
Mechthild Thalhammer, University of Innsbruck, Austria

In this talk, I shall primarily address the issue of efficient numerical methods for the space and time discretisation of nonlinear Schrödinger equations such as systems of coupled time-dependent Gross-Pitaevskii equations arising in quantum physics for the description of multi-component Bose-Einstein condensates. For the considered class of problems, a variety of contributions confirms the favourable behaviour of pseudo-spectral and exponential operator splitting methods regarding efficiency and accuracy. However, due to the fact that in the absence of an adaptive local error control in space and time, the reliability of the numerical solution and the performance of the space and time discretisation strongly depends on the experienced scientist selecting the space and time grid in advance, I will exemplify different approaches for the reliable time integration of Gross-Pitaevskii systems on the basis of a local error control for splitting methods.

The low-barrier problem in long-time atomistic dynamics
Arthur Voter, Los Alamos National Laboratory, USA

Many important materials processes take place on time scales that vastly exceed the nanoseconds accessible to molecular dynamics simulation. Typically, this long-time dynamical evolution is characterized by a succession of thermally activated infrequent events involving defects in the material. Accelerated molecular dynamics methods (hyperdynamics, parallel replica dynamics and temperature accelerated dynamics) and adaptive kinetic Monte Carlo methods, developed over the past 10-15 years, have made significant progress on this problem. These methods evolve the system from state to state in a dynamically accurate way, sometimes reaching time scales orders of magnitude longer than MD can. A significant remaining challenge arises from the fact that the more realistic the system under study, the more likely that many of the processes have low activation barriers, and this characteristic can severely limit the computational boost factor. After an introduction to these long-time atomistic methods, I will discuss some of our latest thinking on ways to mitigate this problem, including the use of the accelerated superbasin kinetic Monte Carlo method [A. Chatterjee and A.F. Voter, J. Chem. Phys., 132, 194101 (2010)] in the context of the accelerated molecular dynamics methods.

On the multi-dimensional compressible Navier-stokes system
Zhouping Xin, Chinese University of Hong Kong, Hong Kong

In this talk, I will discuss some of the recent developments on the global in time existence of classical solutions to the multi-dimensional compressible Navier-Stokes equations for data which may be of large oscillations and contain vacuums. Some new phenomena and analysis will be reported.

Topology and geometry versus atomistics and chemistry of low-dimensional materials
Boris Yakobson, Rice University, USA

To transform a geometrical concept of a line or a plane into a model of material object, one must invoke some basic physical measures, like energy or force. We will discuss how such 'innocuous' model extension inevitably leads to the notion of discrete atom, chemical bond, and all the complexity of quantitative materials science. Illustrations will be 1D-nanowires, nanotubes, polymer chains, or 2D-graphene, h-BN, ribbons, edges and interfaces, mainly from recent research of my group at Rice.

Multiscale methods for elliptic homogenization problems
Xingye Yue, Soochow University, China

In this talk, we will give a short review on multiscale methods for elliptic homogenization problems. We will emphasize the intrinsic links between some popular methods such as generalized .nite element methods, residual-free bubble methods, variational multiscale methods, multiscale .nite element methods and heterogeneous multiscale methods.

Numerical study of phase and phase transition based on nonlinear variation
Pingwen Zhang, Peking University, China

The rich and fascinating phases, resulting from the subtle balance of two or more completing factors, as well as the phase transition in actual condensed physical systems, have been received tremendous attention in scientific community and industry. Some well-known illustrations come from block copolymer systems, liquid crystal systems, electric-carrying systems etc. How to efficiently discover new phases and study their phase translation presents a set of interesting and challenging problems. Mathematically, these problems can be translated into the study of the corresponding nonlinear variation (NV).

In this talk, we focus on the numerical study of the NV, which can be divided into three main parts: the discrete methods, the iterative methods, and the reasonable initial values. The iterative methods are heavily dependent on the mathematical structures of the NV itself. The way of the system modeling will result in different mathematical features of the NV. And the initial values can be screened by the comprehension of physical mechanism. Therefore, solving the NV with profound physical background needs a comprehensive consideration. Lastly, the block copolymer systems are taken as an example to demonstrate the approach. We present a novel self-consistent field theory for general polymeric systems using the Gaussian functional integration technique. It reveals many favorable mathematical features, one of which is that it points out the descent and ascent directions of the effective Hamiltonian. With these properties, a series of gradient-typed algorithms are developed to accelerate the self-consistent field iteration procedure with a careful comparison

with the traditional iterative methods. If time allows, we will show some more results of the discovery of new phases and the ordered nucleation phase transition in block copolymers.

Effective boundary conditions for the Stokes fluid with thin coatings via homogenization

Zheng-An Yao

In this report, we consider a mathematical problem arising from the fluids by applying a thin coat of special area to a body to be protected. The body is assumed to be a 2-Dimensional smooth and bounded region denoted by Ω_1. The thin coat occupies the region

$$\Omega_2 := \{x \in R^2 \setminus \Omega_1 | d(x) < \delta\} \quad \text{where} \quad d(x) := dist(x, \bar{\Omega}_1) = \min_{y \in \bar{\Omega}_1} |x - y|, \quad (1)$$

where δ is the thickness of Ω_2 satisfying $\delta \ll 1$.

We study the Stokes fluid in the coated body

$$\begin{cases} \dfrac{\partial u^\delta}{\partial t} - \mathrm{div}(\mathcal{A}\nabla u^\delta) + \nabla p^\delta = 0, \quad \text{in} \quad \Omega, \\ \mathrm{div} u^\delta = 0 \quad \text{in} \quad \Omega, \\ u^\delta|_{t=0} = u_0^\delta(x), \quad u^\delta|_{\partial\Omega} = 0, \qquad \text{for} \quad t > 0, \end{cases} \quad (2)$$

where u^δ and p^δ are the velocity and the pressure of the fluid respectively. $\mathcal{A}$ is a 2×2 matrix, which is positive and symmetry. It is assumed that the interior body Ω_1 is homogeneous , namely,

$$A(x) = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \forall x \in \Omega_1. \quad (3)$$

Within the coating Ω_2, we assume the tensor $\mathcal{A}$ takes the form

$$\mathcal{A}(x)\nu = \sigma\nu, \quad \mathcal{A}(x)\tau = \mu\tau, \quad \forall x \in \Omega_2, \quad (4)$$

where σ and μ are positive constants, $\nu = \nabla d(x)$ is the unit normal vector and $\tau \perp \nu$ is a unit tangent vector.

Our goal is to find the behavior of u^δ, p^δ as δ tends to zero. We also want to find out the boundary conditions of the effective model.