Numerical Analysis of Multiscale Computations

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Short Overview

With the efficiency of modern computers and the maturity of numerical methods for solving differential equations and linear systems, the focus of scientific computation has recently been shifting towards more difficult problems where classical single physics models are not accurate enough, and a coupling of multiple physics models needs to be considered. In particular, there is an emergence of methods that replace heuristics and empirical observations in coarse scale single physics models by direct numerical simulations of more accurate models defined on finer scales. This workshop addressed the numerical analysis of such multiscale approaches.

As an example, in simulation of complex fluids, such as polymers in a solvent, a coarse scale model is given by Navier-Stokes type PDEs for non-Newtonian fluids. In such a model, the total stress is typically obtained through empirical arguments based on physical insights. The accuracy of the model thus hinges critically on the quality of the heuristics, which is often not satisfactory. In the emerging methods, the total stress could instead be obtained by direct fine scale numerical simulations of the interaction of polymer particles and the background fluid. With these approaches, the resulting models typically require solving problems involving wide ranges in spatial and temporal scales. In fact, one of the main challenges for simulating fine scale models, e.g. molecular dynamics and kinetic Monte-Carlo, lies in computationally resolving details such as oscillations over the length scales, both spatial and temporal, where interesting phenomena take place. It is generally an impossible task to solve the fine scale equations accurately over the length scale of the interesting continuum quantities, and in the time dependent case, for a time scale comparable to that of interesting events.

The new class of numerical methods alluded to above typically tackle this difficulty by exploiting separations of scales or other scale structures such as self similarity in the governing physical model. There is a large class of problems that exhibit this separation of scales — it implies that enough information about the fine scale influence on the coarse scale dynamics can be obtained by performing spatially localized simulations over short times, thus gaining efficiency. The numerical complexity of these methods is therefore expected to be much smaller than direct simulation of the full fine scale model.

This sort of multiscale approach makes it feasible to treat problems that could not be handled previously and to obtain higher accuracy in the simulation of important physical phenomena. So far the main excitement has been driven by multiscale mathematical models in applied sciences problems including materials science, chemistry, fluid dynamics, and biology. In this workshop, the focus was on the analysis of the numerical methods motivated by these attempts.

Objectives of the workshop

Abstractly, the problems we are interested in can be described as follows. A fine scale model for the high-dimensional variables x is known. We want to compute a number of "coarse" variables, X, using a tentative governing equation. Parts of the data in the governing equation is, however, missing and must be constructed from the solutions x of localized simulations of the fine scale model. In those simulations, parameters such as boundary and initial conditions, depend implicitly on the coarse variables X.

A difficulty is how to choose a good coarse model when only the fine scale model is known. The models of each scale can be of different types: e.g. PDEs, ODEs, integral equations, stochastic processes. In many applications, stochastic modeling is more appropriate. The coarse and fine scale models are often not of the same type. For instance, molecular dynamics (ODEs) can be a fine scale model of fluids, while a coarse scale model could be Navier-Stokes (a PDE). Similarly, Monte-Carlo methods can be used either as a valid method for the coarse scale system or used in a fine scale to evaluate coarse scale quantities, while some other type of computational model is used in the complement scale.

There are also situations where there is no explicit equation for the coarse variables, and we are interested in developing direct numerical procedures to consistently drive the coarse scale evolution by using snapshots of fine scale solutions. As an example, the Fermi-Pasta-Ulam problem is to study the adiabatic energy transfer in a system of interlaced linear stiff springs and "soft"' nonlinear ones. The adiabatic energy transfer in the system is an important phenomenon that only professes itself when the energies of the right springs in the original system is explicitly computed. Each spring in the system oscillates at similar fast time scales, and it is not obvious what coarse variable should be used to consistently compute the energy transfer in the system.

Hence, in this workshop we proposed to address the following specialized aspects related to the multiscale computational approaches alluded to above:

1. Under what conditions and in what sense do the multiscale approaches converge (while still having a significantly smaller complexity than that of direct simulation of the fine scale model)? What is the accuracy and the stability properties of the methods?

2. Is the coarse system properly closed, i.e. are the chosen X variables enough to describe the coarse dynamics that is consistent with the fine scale system? If not, what additional auxiliary coarse variables are needed to close the coarse system?

3. How can we find reasonable coarse models in a systematic way? Can numerical methods be used to automate the process?

These pose challenging computational and analytical problems. Some initial work has been done on Item 1 for some classes of methods, but many open questions remain. Item 2 and 3 have been addressed traditionally by applying empirical rules based on physics, theories developed from mathematical physics, such as statistical mechanics, or by rigorous analytical approaches such as homogenization in simplified settings.

Workshop Themes

Coarse variables

One generic difficulty for the new multiscale methods is to chose the coarse, macroscopic variables. The speakers followed different approaches to accomplish this. In the dynamical systems setting Sharp used time averages of the state variables of the given mechanical systems and analyzed how the dynamics of these time averages could possible form a closed system. In LeBris's method the slow variables correspond to the amplitudes of the oscillations. It should be noted also that by choosing a symplectic method the energy is approximately kept constant and can be considered as a coarse variable that is implicitly computed and used. Ariel proposed a systematic way to find slow variables by considering polynomial functions of the fast variables and show that a finite number of such slow variables could result in an effective system which can be considered closed. Ariel further demonstrated the effectively of such multiscale method comparing to some typical test problems such as the Fermi-Pasta-Ulam problem.
Bold considered the distribution function of frequencies as a slow-moving variable.
Vanden-Eijden and Szepessy used statistical properties of the fast variables.

Complexity

One of the main goals of the new multiscale methods is to significantly reduce the complexity compared to solving the full problem. Overall, we see the use of coarse variables and special sampling approaches to breach complexity limitation.
This aspect was highlighted in several talks:

Vanden-Eijnden showed that for a class of stochastic systems for modeling chemical reactions with drastically different rates, one could efficiently simulate the slow reactions without fully resolving all the fast reactions. This is done using a multilevel sampling technique that resembles a recent Monte Carlo algorithm by Petzold ang Gilespy.

Gilbert and Iwen presented an efficient way to identify a few salient Fourier modes in a given signal. This algorithm is based on random sampling theory. For a given error tolerance and probability, the algorithm can return the correct solutions in sublinear time.

The underlying mathematical principle is related to the theory of compressive sensing.

Ariel's talk focused on the idea of searching for a set of functions (slow variables) that changes slowly when evaluated along the solutions of the given dynamical systems with fast oscillation. The time evolution of the slow variables can be computed at a cost almost independent of the fastest scale of the problem.

LeBris used the generating function for a given Hamiltonian system to integrate out the effects of fast harmonic oscillations. The technique suggested provides a way to construct efficient symplectic integrators for the remaining slow dynamics. This is an approach that relies on specific knowledge and theory about the fast oscillations of special systems for breach the limitation of formal complexity.

Luskin analyzed the quasi-continuum model. The efficiency of this algorithm comes from using "coarse-grained" representative atoms and simplified interaction rule (Cauchy-Born) in the bulk of a material (solid) under simulation. The algorithm requires a coupling between the coarse grained bulk and detailed atomistic simulations.

Coupling of models

The challenges of coupling of different models in a multiscale computation are typically about (1) the identification of suitable macroscale or microscale variables; (2) making sure that the mathematical models used in either scales are compatible; and (3) identification of subdomains in which macroscale model are not sufficient and should be replaced by a fine scale model. In particular, the compatibility of the models used at different scales typically involves finding the suitable boundary conditions, for the fine scale domains, that correctly reflect macroscale information, finding the suitable boundary conditions for the macroscale simulations that correctly reflect the effect from fine scale simulations, and setting up the states of the chosen microscale variables which are consistent with the macroscale information.

If some sort of homogeneity in the macro domain is assumed, periodic boundary conditions for the fine scale simulations make sense. Generally speaking, microscale simulations feedback to the macro model through Dircihlet or Neumann type conditions. Initializing the micro variables may be an important issue to resolve.

Ren analyzed different couplings of continuum and atomistic models of fluids by exchanging possible combinations of flux and velocity information in thinly overlapped domains. He analyzed the instability of certain specific coupling methods.

Yi Sun couples a general interface tracking algorithms with Monte Carlo simulations. The MC simulations concentrate on small domains distributed along the interface. Periodic boundary condition is assumed tangential to the interface, and flux type boundary conditions need to be enforced according to macro variables.

Quasicontinuum method uses linear interpolation to couple macro and micro models.

Convergence

Souganidis presented general framework relying on comparison principle for establishing convergence in a numerical method. Luskin proved convergence of the quasicontinuum method in one dimension. Ariel showed that if sufficient number of slow variables is found, then one can construct efficiently convergent numerical approximations of the slowly changing properties of the fast dynamics. Szepessy discussed a hierarchy of stochastics models related to a Langevin dynamics. He proved convergence of one model to the other under certain appropriate scaling. In summary, the residual of the heavy particle's Hamiltonian path in the Kolmogorov equation for Langevin's equation yields a weak error representation. To estimate terms in this representation, the correspondence to the essential martingale property for Ito integrals present in the Langevin dynamics comes here in the Hamiltonian dynamics in more subtly form by Fourier representations based on the first variation of the particle paths with respect to the noisy initial data.

Open Problems and Future Directions

Here, we list a couple of questions that have been raised and discussed during the workshop.

What are the main challenges in multiscale modeling, computation, and analysis?

Is it possible and sensible to develop multiscale approach for phenomena that have many or even a continuum of scales?

For oscillatory problems with time-dependent and crossing eigenvalues, what could be done to overcome the possible singularities that may arise?

In many problems, one should consider even longer time scales (1/eps^2). What are the additional challenges for such considerations? What may be the additional problems for "stacking" the two-scale algorithms?

In deriving macro- models from micro- models that include stochastics, finding good ways of using noise helps in this coarse-graining process.

A hard open problem is to find mathematical methods to derive efficient pseudo-potentials in molecular dynamics. Now, this problem is studied with chemists' and physicists' lifelong experience. It would be helpful to find simpler mathematical ways.

Some discussions on the spectrum of the KdV model took place. The issue of whether using only a few salient Fourier modes in this type of problems is sufficient was raised. More generally, for what type of equation/operator does this approach make sense?

Multiscale problems are also multi-disciplinary, so we need to have more input from experts in other areas. Experts on micro in physics, biology and chemistry should help to give input on our work and show problems where new math is needed.

More problems starting from the Schrödinger equation would be good to have, since this is the model where everything is precisely defined, taking steps into coarser scales from there is interesting.

From purely analytical view point, the passage from molecular dynamics regime to continuum regimes are still unclear.

Participants

Ariel, Gil (University of Texas, Austin)
Bold, Katy (Princeton University)
Engquist, Björn (University of Texas, Austin)
Gamba, Irene (University of Texas, Austin)
Gilbert, Anna (University of Michigan)
Iwen, Mark (University of Michigan)
Le Bris, Claude (CERMICS-ENPC, Paris)
Luskin, Mitchell (University of Minnesota)
Ren, Weiqing (New York University)
Runborg, Olof (Royal Institute of Technology)
Ruuth, Steve (Simon Fraser University)
Sharp, Richard (University of Texas at Austin)
Souganidis, Panagiotis (University of Texas, Austin)
Sun, Yi (New York University)
Szepessy, Anders (Royal Institute of Technology)
Tsai, Richard (University of Texas, Austin)
Tharkabhushanam, Sri Harsha (University of Texas, Austin)
Vanden-Eijnden, Eric (New York University)

Statistics:
Tenured professors: 9
Assistant professors: 3
Post-docs:3
Graduate students: 3

Men: 15
Women:3

Excerpts from the talks (grouped by topics)

Dynamical systems

Speaker: **Ariel, Gil** (University of Texas, Austin)
Title: *Applications of heterogeneous multiscale methods to stiff ordinary differential equations*

This talk focused on a class of ordinary differential equations (ODEs) whose dynamics exhibits oscillatory behavior in two well separated timescales. Ariel proposed a numerical algorithm that consists of two steps. The first identifies a set of variables that characterize the slow dynamics. If a sufficient number of independent variables are found, they serve as a coordinate system for the slow modes of the dynamical system, and consequently, the application of an averaging theorem provides closure to the dynamics. He showed that for a class of equations, including the Fermi-Pasta-Ulam problem, a closed set of slow variables can be constructed by forming the appropriate linear combinations of the monomials of the original state variables.

Speaker: **Bold, Katy** (Princeton University)
Title: *Coarse-graining the dynamics of coupled oscillator models*

Bold presented a multiscale computational approach to study the collective dynamics of Kuramoto model and a model of glycolytic oscillations in yeast cells — these models are used to study coupled transient dynamics and synchronization. The two models of coupled, heterogeneous oscillators we consider are the Kuramoto model and a model of glycolytic oscillations in yeast cells. She pointed out that for these two problems, it is essential to use some appropriate distributions of the state variables on the macroscopic level and to constraint the microscopic simulations. She also discussed the existence and stability of fully and partially synchronized states in these models. Bold also described her approach to a multiscale modeling for the graph problems.

Speaker: **Le Bris, Claude** (CERMICS-ENPC, Paris)
Title: *Construction of symplectic schemes for highly oscillatory hamiltonian systems*

Le Bris described a systematic Hamilton-Jacobi approach to construct symplectic integrators for highly oscillatory systems**.** The approach is based upon a two-scale expansion of the generating function. Some non-symplectic integrators are also constructed, slightly modifying the above strategy. He pointed out that in the context of multiscale applications, symplecticity of a numerical scheme is not the ultimate goals, but the efficiency of this algorithm is. He proposed the idea of partial symplecticity for the slow variables. In parallel to symplecticity, symmetry preservation is also a desired properties. Symmetry in a scheme implies conservation of invariants in the system. He discussed his reflection on whether replacing symplecticity with symmetry in the algorithm would be appropriate for non-integrable systems.

Speaker: **Sharp, Richard** (University of Texas at Austin)
Title: *Systematic reinitialization for heterogeneous multiscale methods*

Sharp used a series of examples, including the problem of Kapitza's pendulum and a chain of molecules in 3D with stiff bonding to illustrate the necessary considerations and approach for designing multiscale algorithms that use the time averages of the state variables as part of the macroscopic variables. Sharp went on to describe how to find the

initial data for the given stiff system so that the averages of the solution using these initial data are consistent with the macroscopic variables. His computations suggested that the preservation of the total energy in these mechanical systems have tremendous consequence for the multiscale simulations. Some questions and discussions followed on his numerical simulations of the Kaptiza's inverted pendulum.

Stochastics systems

Speaker: **Luskin, Mitchell** (University of Minnesota)
Title: *Mathematical results and challenges for the quasicontinuum approximation*

Luskin derived and compared several quasicontinuum approximations to a one-dimensional system of atoms that interact by a classical atomistic potential. He proved that the equilibrium equations have a unique solution under suitable restrictions on the loads, and we give a convergence rate for an iterative method to solve the equilibrium equations.

Speaker: **Szepessy, Anders** (Royal Institute of Technology)
Title: *Stochastic dynamics in atomistic and continuum models*

Stochastic Langevin dynamics is used for simulating molecular dynamics at constant temperature. More than thirty years ago, Robert Zwanzig showed that a Hamiltonian system of harmonic heat bath interactions with particles, for stochastic initial data, can be modeled by a Langevin equation. It is also well known that Langevin dynamics can be approximated by simpler Smoluchowski dynamics (Brownian dynamics) on long diffusion time scales as the molecular friction increase. Szepessy presented some simple ideas and error estimates for coarse-graining:
heat baths to Langevin,
Langevin to Smoluchowski, and
Smoluchowski to continuum stochastic PDE for phase change dynamics.

Speaker: **Vanden-Eijnden, Eric** (New York University)
Title: *Numerical techniques for multiscale stochastic dynamical systems*

Vanden-Eijnden pointed out that traditional implicit ODE schemes become ineffective when the dynamics of the system is stochastic in some way, e.g. if it is governed by a stochastic differential equation, a Markov chain as in kinetic Monte Carlo methods, or even by a large set of ODEs whose solutions are chaotic. He spoke about a type numerical methods that are built on asymptotic techniques and limit theorems for singularly perturbed Markov processes, originally developed in the 70s by Khasminskii, Kurtz, Papanicolaou, etc. These limit theorems provide one with closed effective equations for the slow variables in the system, and the coefficients in these equations are given by expectations over the statistics of the fast variables conditional on the value of the slow variables. In general, these expectations cannot be computed analytically, but it is possible to estimate them on-the-fly when needed via short runs of the fast variables. Once this is done, the slow variables can be evolved using the effective equations by one macro-time-step, and the procedure can be repeated. Vanden-Eijnden carefully compared the differences between the Heterogeneous Multiscale Methods and the

Equation-Free approaches. In this approach, the initial condition for each microscopic run does not seems to be important. This is in contrast to many other problems that were presented in this workshop. There were discussions on how one can set up a model stochastic problem with correlated noise so that certain auxiliary macroscopic variables are indispensable for a consistent multiscale approximation.

Solids and fluids

Speaker: **Ren, Weiqing** (New York University)
Title: *Numerical test of multiscale methods for fluids*

Ren proposed a numerical approach that couples the continuum equations and molecular dynamics over an interface that separate the two models. The boundary condition for the continuum equations at the interface is provided by molecular dynamics, and vice versa. Two crucial problems need to be resolved: 1) what information (macroscopic) needs to be exchanged between the two descriptions? 2) How to impose BCs that are prescribed macroscopically on the particle systems? The second question typically leads to artificial disturbance being reflected from the coupling interface. There was a brief discussion about the approach of overlapping MD and continuum domains for tacking this problem. Ren concentrated on the first question in this talk. In the existing methods, coupling between (a) field functions (e.g. velocity); (b) flux of conserved quantities; and (3) mixture of the above have been proposed, while flux(continuum)-flux(particle) and velocity(continuum)-velocity(particle) are the most popular ones. Ren presented his finding in the performance of these different schemes. He concluded that flux-velocity coupling yields faster convergences than other combinations, flux-flux coupling is marginally unstable, and velocity-flux coupling yields errors that increase geometrically in time.

Speaker: **Sun, Yi** (New York University)
Title: *The heterogeneous multiscale methods for interface tracking*

This talk proposed two integrated multiscale techniques to the simulation of combustion fronts and epitaxial growth. For the application to the combustion fronts the main task is to overcome the numerical difficulties caused by different time scales on the transport part and the reactive part in the model. Sun showed numerical results related to Majda's model and reactive Euler equations in one and two dimensions show substantially improved efficiency over traditional methods. For the epitaxial growth, a hybrid method coupling the kinetic Monte-Carlo simulation on the microscale with the level set method for island dynamics on the macroscale is introduced. Sun further demonstrated the efficiency of his approaches by presenting relevant numerical computations for island growth and step edge in the epitaxial growth model. In both applications, the macroscopic variables include an interface that separates different materials as well as some statistical quantities, such as density of the particles, related to the microscopic state variables. A discussion on the evaluation of the interface dynamics from the microscale simulations, which is typically measured by fluxes of the materials near the interface.

Again it is very important to correctly handle the boundary conditions at each of the microscopic domains. Sun described his approach that set up microscopic domains that are in alignment with the interface normal in order to better derive and enforce the boundary conditions.

Kinetics

Speaker: **Gamba, Irene** (University of Texas, Austin)
Title: *Non-equilibrium statistics and the need of multi scale analysis in heterogeneous modeling for charged transport in nano structures*

Gamba discussed issues of semi-classical and classical kinetic models for hot electron transport in nano channels and their macroscopic limits. Such models depend on the relative effective forces. Gamba also discussed the applicable regimes of the Boltzmann-Poisson and Wigner-Poisson models, which depend on the scales and their macroscopic approximation equations for their kinetic moments. An important issue for the characterization of the multi-scale is the boundary conditions. In addition, she presented some recent deterministic solvers for kinetic equations and benchmark simulations against Monte Carlo solvers for Boltzmann-Poisson systems.

Speaker: **Tharkabhushanam, Sri Harsha** (University of Texas, Austin)
Title: *Deterministic solvers for non-linear Boltzmann equation and computations of non-equilibrium statistical state*

This speaker presented a new deterministic solver for the non-linear Boltzmann Transport Equation (conservative and non-conservative) for Variable Hard Potential (VHP) model. The speaker pointed out that in the Boltzmann collision kernel, the inter-dependence of the pre- and post- collisional velocities and the distribution posses the major computational challenge. Using a Fourier transform technique, the complexity in computing the collision integral is isolated to a separate integral over the unit sphere. The resulting numerical algorithm requires solving a constrained minimization problem in order to achieve conservation of mass. The high-velocity tail behaviour (power-like tails) of the distribution function is captured by the computation of high-order moments of the distribution function.

Novel applications

Speaker: **Gilbert, Anna** (University of Michigan)
Title: *Sublinear algorithms for (sparse) signal representation*

Gilbert gave an expository overview of several sublinear algorithms for sparse signal representation, including the Fourier sampling algorithm of Gilbert, Muthukrishnan, and Strauss. These algorithms are exponentially faster than traditional algorithms and use exponentially less space; some reading only a small fraction of the signal. In exchange for this exponential decrease in resources used, the algorithms are randomized approximation algorithms. She discussed in detail a combinatorial technique, called

group testing, which is an essential step in the new Fourier methods. There are discussions about when these type of random algorithms yield deterministic result.

Speaker: **Iwen, Mark** (University of Michigan)
Title: *Sub-linear time approximate DFT algorithm for spectral methods*

The fast approximate in "Improved time bounds for near-optimal sparse Fourier representation via sampling" will be briefly reviewed. Iwen presented some empirical results on the speed, accuracy, and noise tolerance from the DFT algorithm proposed by A.C. Gilbert, S. Muthukrishnan, and M. J. Strauss. Iwen then focussed on using the algorithm for sub-linear time/space spectral methods for the KdV equations.

Analysis

Speaker: **Souganidis, Panagiotis** (University of Texas, Austin)
Title: *Error estimates for finite difference numerical approximations to solutions of fully nonlinear first and second order PDE*

Souganidis first reviewed the basic convergence theory for monotone finite difference approximations to viscosity solutions and then presented new results about error estimates. The second part of his talk focused on the homogenization of Hamilton-Jacobi equations and degenerate parabolic or elliptic equations in a class of random media. This type of equations is highly related to flow in heterogeneous media in which the heterogeneity is larger than the pore scales. To date, there are very limited computational strategies for this type of problems. Tsai is now interacting with Souganidis and his student on these problems.

Interactions:

A. Discussions and exchanges of ideas:

Runborg, Iwen, and Gilbert discussed a joint project on developing spectral methods for PDEs using the new fast Fourier Transform algorithm.

Sun and Tsai discussed the multiscale modeling and computation for a class of neural networks that involve stiff Dirac-delta forcings.

Engquist, Runborg, and Tsai discussed new numerical approach for high frequency wave propagation using Gaussian beams.

Vanden-Eijnden, Ariel, and Tsai discussed the possibility of improving the convergence of time averaging.

Several discussions on the range of validity of the Cauchy-Born rule following Luskin's talk took place.
LeBris and Sharp discussed the issue of conservation of total energy in his algorithm.

There were discussions on the possibility of adding suitable macroscopic variables could improve the conservations

LeBris and Szepessy started thinking on symplectic methods for optimal control point of view.

Discussions about general approaches in finding coarse variables took place after Bold's talk. Comments about the convergence of the presented graph problem were exchanged.

Ariel, Szepessy, and Vanden Eijnden discussed the issues of strong versus weak convergence of the Zwanzig model to the Langevin equation.

Some discussions on the spectrum of the KdV model presented in Iwen's talk took place. The issue of whether using only a few salient Fourier modes in this type of problems is sufficient was raised. More generally, for what type of equation/operator does this approach make sense?

B. Mutual visits

Tsai visited Luskin at Minnesota after the workshop.

Vanden-Eijnden invited Tsai to a workshop in the summer at St. Malo.

Gilbert and Runborg met in Cambridge and further developed their collaboration.