

Abstracts

A pure streamfunction approach to Navier-Stokes Equations in two dimensions

Matania Ben-Artzi, Hebrew University, Israel

A pure-streamfunction formulation is introduced for the theoretical study and numerical simulation of the 2-D incompressible Navier-Stokes equations. On the theoretical level, it leads to a nonlinear evolution equation involving the bi-laplacian. The basic mathematical results are concerned with the well-posedness of the system subject to "rough" initial data (such as point vortices). For the numerical aspect of the talk, a new compact scheme is presented, which allows for a pure streamfunction formulation, very close to the theoretical treatment. This scheme is robust and, by using only the streamfunction, does not require vorticity boundary conditions (a major difficulty of vortex methods).

The scheme is analyzed for stability and convergence. It is shown to converge for the full nonlinear system. Numerical experiments are presented, including driven and double-driven cavities. For sufficiently high Reynolds numbers, the solution bifurcates, leading to symmetry breaking patterns and periodic solutions. (Joint work with J.-P. Croisille, D. Fishelov and S. Trachtenberg).

Growth and Pattern Formation for Epitaxial Surfaces

Russel Caflisch, UCLA

Growth of an epitaxial thin film involves physics on both atomistic and continuum length scales. For example, diffusion of adatoms can be coarse-grained, but nucleation of new islands and breakup for existing islands are best described atomistically. The lattice properties of the film are determined by those of the underlying substrate. In heteroepitaxial growth, e.g., Germanium on Silicon, mismatch between the lattice spacing of the Silicon substrate and the Germanium film will introduce a strain into the film, which can significantly influence the material structure leading for example to the formation of quantum dots. Techno-logical applications of quantum dot arrays require a degree of geometric uniformity that has been difficult to achieve. One approach to overcoming this difficulty is to prepattern the system, for example with buried dislocation lines. This talk will describe mathematical modelling, simulation methods and computational results for epitaxial growth, strain in thin films and pattern formation. The growth simulations use an island dynamics model with a level set simulation method. Strain computations can be computationally intensive, so that effective simulation of atomistic strain effects relies on an accelerated method that incorporates algebraic multigrid and an artificial boundary condition. Simulations that combine growth and strain will be presented showing spontaneous and directed self-assembly of patterns (quantum dots and wires) on thin films.

Transonic flow, shock reflection, and free boundary problems

Gui-Qiang Chen, Northwestern University

When a plane shock hits a wedge head on, it experiences a reflection-diffraction process and then a self-similar reflected shock moves outward as the original shock moves forward in time. The complexity of reflection picture was first reported by Ernst Mach in 1878, and experimental, computational, and asymptotic analysis has shown that various patterns of reflected shocks may occur, including regular and Mach reflection. However, most fundamental issues for shock reflection have not been understood, including the transition of the different patterns of shock reflection, and there had been no rigorous mathematical result on the global existence and structural stability of shock reflection, especially for potential flow which has widely been used in aerodynamics.

In this talk we will start with various shock reflection phenomena and their fundamental scientific issues. Then we will describe how the shock reflection problems can be formulated into free boundary problems for nonlinear partial differential equations of mixed-composite type. Finally we will discuss some recent developments in attacking the shock reflection problems, including our results with M. Feldman on the global existence and stability of solutions of shock reflection by large-angle wedges for potential flow. The approach includes techniques to handle free boundary problems, degenerate elliptic equations, and corner singularities when free boundaries meet degenerate elliptic curves.

Twist & Shout: Maximal enstrophy production in the 3D Navier-Stokes Equations

Charles R. Doering, University of Michigan at Ann Arbor

It is still not known whether solutions to the 3D Navier-Stokes equations for incompressible flows in a finite periodic box can become singular in finite time. (Indeed, this question is the subject of one of the \$1M Clay Prize problems.) It is known that a solution remains smooth as long as the enstrophy, i.e., the mean-square vorticity, of the solution is finite. The generation rate of enstrophy is given by a functional that can be bounded using elementary functional estimates. Those estimates establish short-time regularity but do not rule out finite-time singularities in the solutions. In this work we formulate and solve the variational problem for the maximal growth rate of enstrophy and display flows that generate enstrophy at the greatest possible rate. Implications for questions of regularity or singularity in solutions of the 3D Navier-Stokes equations are discussed. This is joint work with Lu Lu (Wachovia Investments).

Quadrature-based moment methods for Boltzmann-like equations

Rodney O. Fox, Iowa State University

In complex multiphase system, polydispersity can arise in many different forms. For example, particle-size distributions in gas-solid flow or bubble-size distributions in gas-liquid flow are two common forms of polydispersity. In general, polydispersity in a multiphase flow will lead to dynamic effects because the interphase momentum transfer terms depend on particle size (or Stokes number). These effects can be accounted for by solving a Boltzmann-like transport equation for the number density function (NDF), which represents the average number density of particles with a given set of properties (e.g., velocity, size, concentration, etc.) Perhaps the most well-known equation of this type is the kinetic equation for the particle velocity distribution function (e.g. the Boltzmann equation), and its extension to include drag and collisions for dilute gas-solid flows.

Solving a Boltzmann-like transport equation for the NDF is non-trivial due to the large number of degrees of freedom. In the literature, the two most popular approximation methods are the Euler-Lagrange method, which treats the dispersed phase as an ensemble of statistical “particles”, and the Euler-Euler method, which solves for the moments of the NDF. In principle, both methods should yield the same predictions for the moments of the NDF. However, this is usually not the case due to differences in the moment closures applied at the level of the Euler-Euler description. Paradoxically, the differences between the Euler-Lagrange and Euler-Euler methods are greatest for what would appear to be the simplest case: dilute gas-solid flow with moderate to large Stokes numbers.

Quadrature methods treat polydispersity by representing the moments of the NDF by a finite set of weights and abscissas. By using the one-to-one correspondence between a set of $2N$ moments and the N weights and N abscissas, the moment transport equations are closed and can be solved to any desired degree of accuracy (which is determined by the choice of N .) In this talk, we will discuss the basic implementation of quadrature methods starting from a Boltzmann-like transport equation for the NDF, and show how they overcome the difficulties associated with “standard” Euler-Euler moment closures. Examples taken from gas-solid flow at finite Stokes number will be used to illustrate the approach.

Shape optimization for eigenvalue problems and applications to photonic crystals and vibrating systems

Chiu-Yen Kao, Ohio State University

Identification or optimization of shapes arises in many science and engineering applications. Recently shape derivatives and topological derivatives have been incorporated into level set method to study inverse problems involving shapes. This talk will provide an integrated introduction to the definition of shape derivatives and topological derivatives, and the combination with level set methods in a descent framework. Finally, specific applications for identifying shapes of drums, maximizing photonic bandgaps and optimizing quality factor are presented.

Coarse-grained computation

Yannis Kevrekidis, Princeton University

The Kevrekidis group explores a framework for computer-aided multiscale analysis, which enables models at a "fine" (microscopic/stochastic) level of description to perform modeling tasks at a "coarse" (macroscopic, systems) level.

In traditional modeling, macroscopic equations are first derived from microscopic models, and then analyzed with available continuum methods. Our equation-free (EF) approach bypasses the derivation of macroscopic evolution equations, provided these equations conceptually exist but are not available in closed form. The mathematics-assisted development of a computational superstructure enables alternative descriptions of the problem physics (LB, KMC, MD, BD microscopic simulators), executed over relatively short time and space scales, to perform systems level tasks (integration over relatively large time and space scales, "coarse" bifurcation analysis, but also optimization and control tasks) directly.

The evolution of a crystal surface below the roughening temperature

Robert V. Kohn, Courant Institute, NYU

Below the roughening temperature, a corrugated crystal surface develops facets at its peaks and valleys. The facets grow and merge, producing a uniformly flat surface in finite time. A widely-accepted PDE model for this process is "motion by surface diffusion" with a convex but non-smooth surface energy like $\int |\nabla_x h| + |\nabla_x h|^3$. This amounts to a highly nonlinear fourth-order parabolic PDE for the surface height $h(x,t)$. I'll discuss recent work with Irakli Odisharia, concerning:

- (i) a robust numerical scheme for computing the evolution of h ; and
- (ii) an explanation why the evolution is asymptotically self-similar.

The physical correctness of this PDE model remains uncertain. A natural approach would be to take the continuum limit of a step-flow model. I'll discuss briefly our (incomplete) understanding of this limit.

Iterative solution methods, error estimation, and atomistic-continuum adaptivity for the quasi-continuum approximation

Mitchell Luskin, University of Minnesota

The quasi-continuum (QC) method has been successfully used to efficiently couple atomistic and continuum models for crystalline solids. The atomistic model is used in regions with highly non-uniform deformations such as around dislocations, whereas the continuum model is used in regions with nearly uniform deformations to give an efficient computation of the energy by reducing the number of degrees of freedom by mesh coarsening.

We give an analysis for a one-dimensional model proving that the equilibrium equations for the QC approximation have a unique solution under suitable restrictions on the loads (less than the limit load), and we give a convergence rate for an iterative method to solve the equilibrium equations.

The quasicontinuum methodology involves the application of the Cauchy-Born rule to the underlying lattice in continuum regions. The validity of this approximation is dependent on the utilization of a unit cell that does not restrict possible lattice instabilities. At the same time, the computational efficiency of the method relies on the use of a minimal cell size. We describe recent work on the development and analysis of an adaptive algorithm to change the element cell size as the element strain evolves during a quasi-static process.

We also develop an a posteriori error estimator which quantifies the modeling error for a goal function and allows for an adaptive decision about which regions should be modeled as a continuum and which regions should be modeled atomistically. We employ the framework of duality based error estimators to measure the approximation error to be minimized in terms of a user-definable goal function.

Joint with Marcel Arndt, Matthew Dobson, Ryan Elliott, and Ellad Tadmor

Some results from the analysis of LSW and one-dimensional coarsening models

Robert Pego, Carnegie Mellon University

I plan to discuss some insights gleaned from recent analysis of some simple but fundamental models of domain coarsening. In particular, gradient structure plays an interesting role for LSW models, for proving optimal well-posedness results, to establish bounds on coarsening rates by the Kohn-Otto method, and prospectively in dealing with corresponding monopole models. And, for a classic model of coarsening in the one-dimensional Allen-Cahn equation, by collapse of smallest domains, a strong analogy to Smoluchowski's coagulation equation is used to establish an optimal well-posedness result and provide necessary and sufficient conditions for the existence of self-similar limits.

Bending back light: The science of negative index materials

Costas M. Soukoulis, Ames Lab/ISU Physics Department

The possibility of negative refraction has brought about a reconsideration of many fundamental optical and electromagnetic phenomena. This new degree of freedom has provided a tremendous stimulus for the physics, optics and engineering communities to investigate how these new ideas can be utilized. Many interesting and potentially important effects not possible in positive refracting materials, such as near-field refocusing and sub-diffraction limited imaging, have been predicted to occur when the refractive index changes sign. In this talk, I will review our own work on negative refraction in metamaterials, and describe the possible impact of them as new types of optical elements. In particular, I will present theoretical and experimental results on engineered microstructures designed to have both ϵ and μ negative. Results for different polarizations and propagation directions will be presented. Recent results on microstructures operating at 100-200 THz and optical wavelengths will be also discussed.

Quantum-size effects in thin film evolution

Cai-Zhuang Wang, Ames Lab

Background (not an abstract): About a decade ago, quantum size effects (QSE) were discovered in metal films on semiconductor surfaces as manifested by perfectly flat films with selected 'magic' thicknesses. This selected morphology reflects compatibility between the wavelength of the electrons in the film and its thick-ness leading to energy minimization. QSE have novel consequences not just for film growth morphologies, but also for post-deposition coarsening of arrays of flat-topped mesa-like islands formed during deposition.

Computational Fluid Dynamics: An implicit P-multigrid approach for the spectral difference method on unstructured grids

Z-J Wang, ISU Aerospace Engineering

A p-multigrid (p = polynomial degree) algorithm is investigated as a solution approach for the spectral difference (SD) method solving the compressible Euler equations on unstructured grids. An implicit non-linear lower-upper symmetric Gauss-Seidel (LU-SGS) relaxation approach is employed as an iterative smoother. In addition, the LU-SGS approach is compared to an explicit TVD Runge-Kutta smoother in terms of performance. Several benchmark test problems are computed, and the new implicit p-multigrid solution approach is one to two orders faster than the explicit Runge-Kutta approach.

Estimates for degenerate equations

Lihe Wang, University of Iowa