Math 273A: Scientific Computation

Fall quarter, 2005

TOPICS IN APPLIED MATHEMATICS AND COMPUTATIONAL SCIENCE

1:00 pm – 1:50 pm, MWF, AP&M 5829

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COURSE ANNOUNCEMENT

In recent years, there have been growing needs and interests in developing mathematical theories and numerical methods for problems arising from materials science, quantum chemistry, biophysics, and many other areas of science. In this research oriented course, we will introduce some of these powerful theories and methods, and demonstrate how they can be applied to the effective modeling, simulation, and analysis of important scientific problems, such as fluid interactions, composites, crystalline defects, phase transitions, surface growth, bio-membranes, electrostatic forces, and electronic structures.

Topical lectures will often begin with a description of the physical phenomenon and experimental results, followed by the derivation of models and analysis of solutions, as well as the presentation of numerical algorithms and simulation results, and conclude with proposals of potential research projects. Students are strongly encouraged to actively participate in class discussions and to give informal presentations on their related researches.

The following is a tentative list of topics that will be partially covered in the course:

1. **Multiscale Methods**
   - The quasi-continuum method for material defects in solids, numerical analysis.
   - Examples of the heterogeneous multiscale method: stiff systems of ordinary differential equations for chemical reactions; homogenization for composites and flow in a porous medium; molecular dynamics and continuum simulation of solids.
   - A coupled molecular dynamics and continuum model for contact lines in fluids, from no-slip to Navier to generalized Navier boundary conditions, negative kinetic constants.
2. **Interface Dynamics**
   - Examples: geometric motions; solidification; epitaxial growth of thin films; microstructural evolution; two-phase flow; and motion of biomolecules.
   - Sharp interface models. The front-tracking method, application to the surface evolution of solid films with dislocations. The level-set method: a simple example. A finite-element level-set method for the stress-driven interface motion.
   - Phase-field models and numerical methods, time stepping, stability beyond the Gronwall inequality, threshold dynamics.
3. **Energy Minimization**
   - Concept of free energy, basics of thermodynamics, the second law.
   - Examples: nonlinear elasticity; the Ginzburg-Landau functional for superconductivity; the Cahn-Hilliard functional for phase separation; the Poisson-Boltzmann model; the Helfrich membrane energy; and the density-functional theory.
   - Weak convergence methods, Γ-limits as effective energies, energies of martensitic thin films.
   - Variational methods for coarsening in gradient systems, application to the coarsening in epitaxial growth of thin films with or without slope selection.
   - The Poisson-Boltzmann model and its improvement, boundary-value problems.
   - The basics of the density-functional theory, the Kohn-Sham equations, real-space calculations using parallel adaptive finite-element methods.

For more information related to this course, such as detailed syllabus, references, potential research projects, and even possible financial support for a Ph.D. thesis project, please contact the instructor, or visit the course web page at http://www.math.ucsd.edu/~bli/teaching/math273Af05/.