STEVENS
Institute of Technology

Seminar Series in Applied Mathematics

Professor Marc Mansfield

Department of Chemistry and Chemical Biology
Stevens Institute of Technology

Solving Laplace's Equation and the Navier-Stokes Equation for Bodies of Arbitrary Shape

Thursday, November 16, 2000
3:15 pm
Morton 103

Abstract: Because of analogies between electrostatics, hydrodynamics, and the statistics of random walks, it is now possible to obtain accurate estimates of the electrical capacitance and polarizability of perfectly conducting particles, or the translational friction coefficient and "intrinsic viscosity" of suspended particles, even when the particles have complex shapes, by simulating the trajectories of random walks in the space surrounding the particle. The analogies arise because the diffusion equation governing the statistics of random walks (when integrated over all times) and an "angular-averaged" version of the Navier-Stokes equation both become equivalent to Laplace's equation. (In the case of the Navier-Stokes equation the analogy is not exact, so hydrodynamic properties calculated in this way are subject to errors of a few percent.) Previously, solutions were typically obtained by finite-element calculations, and were therefore difficult to obtain with accuracy unless the particle had a relatively simple shape. The technique has been validated on a number of simple shapes (spheres, cubes, cylinders, regular polyhedra, tori, etc.) for which exact or accurate numerical results are available, and then applied to macromolecules of extremely complex shape.

Refreshments will be available starting at 3:00pm.

For additional information contact Patrick Miller (216-5452) or Yi Li (216-5433).