# PROPOSAL FOR MATH 728D, SELECTED TOPICS IN APPLIED MATHEMATICS

**Instructor: Daniel Dix.** 777-4320, dix@math.sc.edu

**Subtitle: Numerical Simulation of Biomolecular Systems.**

**Prerequisites.** Undergraduate numerical analysis, ordinary differential equations, linear algebra, probability theory, and functional analysis. No chemistry knowledge will be assumed.

**Textbook.** *Understanding Molecular Simulations: From Algorithms to Applications*, D. Frenkel, B. Smit, Academic Press, 1996. Other references will be provided.

**Topics to be Covered: (as much as possible of the following).**

(1) Numerical methods for large Hamiltonian systems of ODEs
(2) Computation of molecular force fields, CHARMM and AMBER
(3) Boundary conditions
(4) Setting up a simulation in NAMD
(5) Assessing simulation results using VMD
(6) Internal coordinate dynamics
(7) Dynamics with bond lengths and angles frozen.
(8) Stochastic differential equations
(9) Statistical mechanical ensembles
(10) Parallelization

**Discussion.** A very important technique in the modern study of molecular biology and physical biochemistry is that of direct all-atom numerical simulation. This course provides an introduction to the numerical methods involved as well as giving the student hands on experience with simulations of real biomolecular systems, such as various combinations of proteins, nucleic acids, carbohydrates, and/or lipids in water. All-atom numerical simulations challenge the capabilities of computers because accurate force fields are so expensive to compute for systems involving a realistic number of atoms (at least $10^3$), and bond length vibrations occur at very high frequencies, necessitating time steps of the order of a femtosecond, $10^{-15}$ second. But the most biologically interesting events require about 1 second, or $10^{15}$ time steps! This sort of calculation is not feasible with today's computers, so we will also discuss approximations which are designed to reduce the amount of calculation needed. Since the system simulated is highly chaotic, a particular trajectory over a reasonable time interval cannot be reliably computed. However the computed trajectories are believed to yield true statistical information about the actual trajectories. Thus we will also discuss some basic ideas in statistical mechanics.