

SYLLABUS FOR NUMERICAL SIMULATION OF BIOMOLECULAR SYSTEMS, FALL, 2001

Subtitle. Math 728B, Selected Topics in Applied Mathematics

Instructor. Daniel Dix, dix@math.sc.edu, <http://www.math.sc.edu/~dix>.

Office, Phone, and Office Hours. LeConte 400E. 777-4320. By appointment: see me before or after class, call or e-mail to set one up.

Time and Place. MWF 10:10–11:00, LC 316.

Text. *Understanding Molecular Simulation, From Algorithms to Applications*, by Daan Frenkel and Berend Smit, Academic Press, San Diego, 1996. This book describes most of the algorithms and discusses the relevant physics, but proves no theorems. See also *Molecular Modelling, Principles and Applications*, second edition, by Andrew R. Leach, Prentis Hall, London, 2001; and *Computer Simulation of Liquids*, by M.P. Allen and D.J. Tildesley, Oxford University Press, New York, 1987. A large amount of supplementary references and notes will be provided.

Software. We will use free programs: NAMD for molecular simulations, VMD, for analysis and visualization of the results, and RASMOL (version 2.7.2.1 for Unix), which can also be used for molecular visualization. MATLAB (not free, but on the math computers), can be used for general purpose computing. A new program, IMIMOL, will be provided to facilitate molecule building and manipulation. The newest unix versions will be available on the instructor's website. Each student will receive an account on the SUNs in the Mathematics Unix lab.

Homework. Homework will be assigned occasionally, in support of the lectures. The solutions should be carefully written up and turned in when due. They will be graded and returned. Some of the problems will involve computations.

Computing Projects. Each student will also do a more involved computation using NAMD. The details of this project will be described later.

Exams. There will not be any.

Grading. The homework will count two thirds and the computing project will count one third of the final grade.

Continuation in the Spring. Because of the large number of nontrivial topics to be addressed, it is very likely that there will be a continuation of the course during spring semester of 2002.