SYLLABUS FOR BIOMOLECULAR GEOMETRY, SUMMER II, 2001

Instructor. Daniel Dix, 7-4320, dix@math.sc.edu, http://www.math.sc.edu/~dix.

Subtitle. Math 728A, Selected Topics in Applied Mathematics

Time and Place. MTWTh 10:30–12:45, LC 405.

Text. *Molecular Modelling, Principles and Applications*, second edition, by Andrew R. Leach, Prentis Hall, London, 2001. This book provides background knowledge, but little mathematics. A large amount of supplementary references and notes will be provided.

Software. A new program, IMIMOL, will be provided to facilitate molecule building. The newest versions will be available on the instructor's website. A free program, RASMOL, will be used for molecular visualization. Other free programs will be used as well. See the above website for details. Each student will receive an account on the PCs in COSM labs.

Homework. Homework assignments will be assigned most every day, and are due the third class meeting after they are assigned. The solutions should be carefully written up and turned in when due. They will be graded and returned.

Molecule Collections/Building Projects. Each student will build a virtual 3D model of each of a list of biomolecules (to be distributed) and store the .imi, .zmat, .lbl, and .spt files in well-organized hierarchical directories on a floppy disc. There will also be a macromolecular building project which should also be stored on the same floppy disc. This will be turned in on August 10, during the scheduled final exam time.

Grading. The homework, the molecule collection, and the building project will each count one third of the final grade.