ANNOUNCEMENT FOR MATH 728A, SELECTED TOPICS IN APPLIED MATHEMATICS, SUMMER II, 2001

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Subtitle: Three Dimensional Geometry of Biological Molecules.

Prerequisites. Undergraduate linear algebra, advanced calculus. Elementary computer programming. No previous knowledge of chemistry or biology will be assumed or required. Interest in 3D geometry, and the building and visualization of virtual structures in the computer will be very helpful.

Textbook. *Molecular Modelling: Principles and Applications*, Andrew R. Leach, Longman Press, 1996. Other references will be provided.

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

(1) Mathematical description of 3D molecules.
(2) Building molecular assemblies in virtual 3D space.
(3) Systems of polynomial equations, implicit functions.
(4) Regular structures in protein molecules, e.g. α-helices and β-sheets.
(5) Geometry of flexible molecular rings, pseudorotation.
(6) Nucleotides and the double helix structure of DNA.
(7) Sugar molecules and the structures of starch and cellulose (sugar polymers).
(8) Docking two 3D molecules, e.g. an α-helix and bDNA.
(9) Geometry of solid and liquid water, hydrogen-bonding networks.
(10) Phospholipids and lipid bilayer membrane structures.

Discussion. Almost everybody has seen a (probably oversimplified) picture of the double helix structure of DNA, and heard about genes, and Dolly the cloned sheep. But it is less widely known that the molecules out of which living things are built adopt many beautiful and mathematically fascinating shapes in three dimensional (3D) space. This course provides an introduction to the mathematical tools used to describe and manipulate these shapes, as well as giving a "hands on" introduction to the basic molecules of life, from a geometric point of view. Applied mathematics students may enjoy exposure to a new and wide open research area. Biochemistry and/or bioinformatics students will gain a deeper understanding of some of the biomolecules they study in the laboratory, and will be equipped to engage in deeper conformational analyses related to their research. Each student will build, atom by atom, virtual computer models of all the molecules/assemblies covered, and will visualize them using computer graphics programs. Grades will be based on homework assignments and the outcome of these model building projects.

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