Time & Place: TR 3:30–4:45, Education 128

Instructor: Dr. Glenn Williams
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Textbook: Molecular Modeling and Simulation, Tamar Schlick

Course Overview:

This course is intended to provide an introduction to advanced applied mathematical methods including numerical methods for nonlinear optimization, global optimization methods, and numerical methods for solving differential equations. The molecular modeling application will be used as a basis for demonstrating and testing the methods presented. Project work will expose students to computational mathematics through C programming in the UNIX environment.

Prerequisite: Math 312, Math 316U

Grading:

Grades will be determined by three computer modeling projects. Each project will consist of implementing a numerical method to solve a problem in molecular modeling. Students will be allowed to work in groups of two.

Last Day to Withdraw: March 18 (Tue)
Course Topics:

Basic Molecular Biology
Fundamentals of Nucleic Acid and Protein Three-Dimensional Structure
Introduction to Biological Databases
Molecular Mechanics, Force Fields, and Effective Molecular Energy
Molecular Modeling by Minimization of Effective Molecular Energy
Molecular Modeling by Least Squares of Residuals
Newton’s Method for Unconstrained Nonlinear Optimization
Conjugate Gradient Method
Quasi-Newton Methods
Line Search and Trust Region Methods
Global Optimization
Simulated Annealing
Monte Carlo Techniques
Fundamentals of Molecular Dynamics
Introduction to Numerical Methods for Molecular Dynamics Simulations