Molecular Modeling and Visualization

January 2008

Instructor: Jonathan Smith
Office: Nobel 107B
Phone: 933-7321
Email: jmsmith@gustavus.edu
Website: www.gac.edu/~jmsmith

Tuesday, Wednesday, Thursday, Friday 10:30 –12:30
Computer "laboratory" time: TWRF 1:30 – 3:00 PM

Overview:

This project-based course will introduce the concepts and tools of molecular modeling and provide the opportunity to explore the use of these methods in a range of chemical and biochemical research areas. The course will be initiated with a discussion of the use of the available modeling tools, molecular visualization tools, computer resources including the new chemistry supercomputer, and an introduction to the use of Linux, an important background for students with interest in advanced applications. Interdisciplinary examples will be used throughout the course with an emphasis on projects. Theory and concepts will be amplified as individual projects proceed.

Text:

Molecular Modeling: Basic Principles and Applications, Hans-Dieter Holtje and Gerd Folkers, VCH Publishers Inc, 1996.

Exploring Chemistry with Electronic Structure Methods, 2nd Edition, James B. Foresman and Aileen Frisch, 1996.

Assignments:

- *Computational Web page* complete with detail of all projects and separate daily BLOG.
- *Final Poster Presentation* Nobel Lobby on last week
- *Class presentations* on projects and other topics three times
- *Quiz* once on Friday of second week

Participation:

Class discussion and laboratory work will play an integral role in the course and thus the quality of the discussion is dependent on preparation for each class period.

Molecular Modeling and Visualization
January Term 2004

Topics:

Molecular Modeling overview
Linux Introduction: Web pages and more
Modeling small molecules: Gaussian 03
Visualizing small molecules
Biological molecules
Conformational flexibility
Advanced Visualization
Computational Cluster Architecture: getting the job done
Modeling large molecules: Classical molecular mechanics
Molecules in solution: implicit and explicit
Molecules in motion: molecular dynamics and molecular movies…

Grading:

Participation (class discussion, attendance)	50
Web page and WeBLOG: Examined, critiqued, and graded: each Friday 5 PM	4 x 50 = 200
Quiz: Friday 16 10:30 AM	25
Poster	50
Presentations: (3)	3 x 25 = 75
	400