BIOL 7110 / BIOL 4105 / CHEM 4804 / CHEM 8901
Spring, 2012

Course Syllabus

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Office hours: Monday 4–5, or by appointment

Course objectives:

- Give students practical experience in building and evaluating molecular models
- Give students a thorough understanding of the basic principles behind molecular mechanics force fields and algorithms
- Give students practical experience in molecular graphics, energy minimization and molecular dynamics
- Deepen students' understanding of principles of macromolecular structure and dynamics, and of macromolecular structure–function relationships

The course consists of lectures, laboratory exercises, discussion sections, written examinations, and a term project. The last part may include a term project and/or papers from the literature. Students registered for graduate credit will do a few more assignments than those registered for undergraduate credit.

Texts:

There is no required text. You may find one or more of the following to be helpful:

Molecular Modelling for Begineers (Also available for the kindle)
Alan Hinchcliffe (John Wiley, 2003)
Hinchcliffe's book is an introductory text, covering both molecular mechanical models and quantum mechanics models, with an excellent appendix covering basic math. *Recommended*.

Molecular Modelling: Principles and Applications, Second Edition
Andrew R. Leach (Prentice–Hall, 2001)
Leach's book emphasizes the thermodynamic and statistical mechanical basis of simulations and covers both molecular mechanical methods and quantum mechanical methods. *Recommended for those with advanced backgrounds in physical chemistry and statistical mechanics*.

Molecular Modeling and Simulation: An Interdisciplinary Guide, Second Edition
Tamar Schlick (Springer, 2010)
A large part of Schlick's book is devoted to molecular structure, and to the motivations for modeling studies. It has an excellent coverage of molecular mechanics methods, with emphasis on algorithms. *Recommended for mathematicians and computer scientists*.

Grading:

Exam 1	20%
Exam 2	20%
Pop quizzes, homework, lab exercises and classroom participation	20%
Final Project	40%
TOTAL	100%

General policies:

Attendance is mandatory at all classes.

Students are allowed one unexcused absence during the semester.

Each additional unexcused absence will result in loss of one full letter grade from the "Classroom Participation" grade

Late homework and lab work will not be accepted, since these are tightly coupled to lectures and discussions, and since the results are presented and discussed in each class where these assignments are due.

Makeup exams: there will be no makeup exams.

Exceptions:

In exceptional cases (*e.g.,* for a student making a presentation at a scientific meeting), I may be persuaded to allow someone to take a makeup exam, but only if it is arranged at least 48 hours before the exam.

Any of the above requirements can be waived in case of: (1) serious illness or injury; (2) the death of a family member; or (3) the serious illness or injury of a partner or a dependent child.

Honor Code:

I take intellectual honesty very seriously, and any violation of the conditions below will result in immediate expulsion from the course with a grade of "F".

– Stephen C. Harvey

I. In order to truly understand the material you are studying, and in order to avoid any student taking unfair advantage of any other, it is absolutely essential that none of you copy or use the results of any one else's work. Throughout most of the semester, you will be encouraged to collaborate with one another, and the free exchange of information and ideas is encouraged, but you are required to complete all assignments yourself. All quizzes and exams must, of course, be completed without consulting anyone else or using any unauthorized materials ("cheat sheets").

II. All students in this course are bound by the conditions of the Georgia Tech Honor Code. A copy of the Honor Code can be found at http://www.deanofstudents.gatech.edu/Honor. The Graduate Appendix to the Honor Code is of sufficient importance that a copy of it is appended here:

Graduate Appendix to the Honor Code

1. Preamble: The Honor Code recognizes that graduate students are involved in research and scholarly activities which occur outside the classroom. Integrity and academic honesty are as fundamental to research and scholarly activity as they are to classroom activity. Therefore, this Appendix to the Honor Code is adopted to pertain to the academic activities of graduate students which occur outside of the classroom.

2. Scholarly Misconduct: Scholarly misconduct refers to misconduct which occurs in research and scholarly activities outside of the classroom. It can include plagiarism, among other things. The consequences of scholarly misconduct are governed by Institute policy. The following definitions are taken from the Institute's Policy on Scholarly Misconduct.

"Misconduct" or "scholarly misconduct" is the fabrication or falsification of data, plagiarism, or other practice that seriously deviates from those that are commonly accepted within the academic or research community for proposing, conducting or reporting research or scholarly activity. It does not include honest error or honest differences in interpretation or judgments of data.

"Plagiarism" is the act of appropriating the literary composition of another, or parts or passages of his or her writings, or language or ideas of the same, and passing them off as the product of one's own mind. It involves the deliberate use of any outside source without proper acknowledgement. Plagiarism is scholarly misconduct whether it occurs in any work, published or unpublished, or in applications for funding.

Allegations involving scholarly misconduct fall under the Institutes Policy on Scholarly Misconduct. This document details the procedures involved with reporting allegations and with the handling of cases. All graduate students are encouraged to become familiar with this policy, which is available from the Office of the Provost.

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Schedule for Spring, 2012

Students will spend the last ~1/3 of the course working on term projects. During that period, there will also be some lectures and discussions on advanced topics. The exact topics for that period will depend on student interests, and they will be determined after the second exam.

Class	Date	Sections & Topics	Assignment (due next class)
1	Jan 10	Course introduction and overview Units; historical perspective	HW: Units
2	Jan12	Macromolecular structure; coordinate systems; conformational space; degrees of freedom	HW: Structure & coordinate systems
3	Jan 17	Thermodynamics I: The first law; thermochemistry	HW: Thermo 1
4	Jan 19	Thermodynamics II: The second law; entropy; free energy; equilibrium; Boltzmann relationship; binding reactions	HW: Thermo 2
5	Jan 24	Thermodynamics III: Thermodynamic cycles; multiple equilibria; ensembles; thermodynamics and life; thermodynamics and molecular modeling	HW: Thermo 3
6	Jan 26	Classical electrostatics	HW: Electrostatics
7	Jan 31	Review; Introduction to VMD	Install VMD and do tutorial (due Feb 7)
8	Feb 2	**Exam I**	

9	Feb 7	VMD; Algorithms I: Newton's equations; harmonic oscillator; molecular dynamics; leapfrog; Energy functions I: Lennard-Jones potential; Oscar; LJ2 tutorial (in class)	Oscar: LJ10 NVE
10	Feb 9	Algorithms II: Optimization & minimization; steepest descent	Oscar: LJ10 minimization
11	Feb 14	Algorithms III: Multiple minimum problem; conformational searches; simulated annealing with MD and MC	Oscar: LJ10 optimization in 2D & 3D
12	Feb 16	Energy functions II: Overview; bonds; angles; torsions; Oscar structure file; Algorithms IV: normal mode analysis	Oscar: Ethane MD
13	Feb 21	Energy Functions III: Electrostatics; improper torsions; other terms; force field parameterization	Oscar: Potential of mean force
14	Feb 23	Simulations I: Introduction; NAMD installation; setting up a simulation; parameter, topology and PSF files	NAMD: Running a simulation
15	Feb 28	Simulations II: Solvation; water models; nonbonded cutoffs; pair lists; repeating boundary conditions; heating, equilibration and production	NAMD: TBD
16	Mar 1	Analysis I: Comparison and evaluation of models: molecular surfaces; contact maps; superposition and RMSD	NAMD: TBD
17	Mar 6	Review; selection and discussion of projects	
18	Mar 8	**Exam II**	
19	Mar 13	Projects and advanced topics	
20	Mar 15	Projects and advanced topics	
Mar 19-23		***Spring Break***	

21	Mar 27	Projects and advanced topics	
22	Mar 29	Projects and advanced topics	
23	Apr 3	Projects and advanced topics	
24	Apr 5	Projects and advanced topics	
25	Apr 10	Projects and advanced topics	
26	Apr 12	Projects and advanced topics	
27	Apr 17	Projects and advanced topics	
28	Apr 19	Projects and advanced topics	
29	Apr 24	Projects; The future of computational structural biology	
30	Apr 26	**Project presentations**	