Conditions of enrollment: Prerequisite: ITSC 8202: Computational Structural Biology.

Course description: This course will cover: (a) overview of statistical mechanics; (b) molecular mechanical force fields; (c) energy minimization and grid search techniques; (d) dynamics simulations (molecular and coarse-grained); (e) Monte-Carlo methods; (f) classical representations of electrostatics (Poisson-Boltzmann, generalized Born, and Coulombic); (g) Brownian dynamics simulation methods; and (h) the distance constraint model.

Learning Objectives of the course: Once completed, students will be able to: (a) understand basic biophysical theories; (b) determine which theory is appropriate for domain specific problems; (c) describe common algorithmic implementations of each method; and (d) apply common implementations of the methods.

Academic integrity: All students are required to read and abide by the Code of Student Academic Integrity. Violations of the Code of Student Academic Integrity, including plagiarism, will result in disciplinary action as provided in the Code. Definitions and examples of plagiarism are set forth in the Code. The Code is available from the Dean of Students Office or online. A set of links to various resources on plagiarism and how to avoid it is available at the UNCC Library website.


Cell phones/pagers: Interruptions to class by cell phones will not be tolerated.

Instructional methods: This course will be based on a mix of traditional lecture format (using the blackboard) and PowerPoint presentations. All PowerPoint presentations will be available on the web at the course website.

Getting help: My office hours are “by appointment”.

Attendance: There is no attendance policy; however, I will be less willing to assist outside of class those students that do not attend.

Grading: Students will be evaluated in the following manner: 30% mid-term exam; 30% final exam; 20% lab exercises; and 20% homework. Grades will be based on 10% increments (i.e. 90-100% = A; 80-89% = B; 70-79% = C; < 70% = U).

1 http://www.legal.uncc.edu/policies/ps-105.html
2 http://library.uncc.edu/display/?dept=instruction&format=open&page=920
Course website: http://www.cs.uncc.edu/~drlivesa/ITSC8311.html

Course outline:

*Week 1-2:* Statistical mechanics overview  
*Week 3-4:* The distance constraint model  
*Week 5:* Overview of molecular mechanical force fields  
*Week 6-7:* Energy minimization and systematic conformational analysis (grid searches)  
**First exam:** End of week 7  
*Week 8-9:* Dynamics simulations (molecular and Go-like)  
*Week 10-11:* Monte-Carlo methods  
*Week 12-13:* Continuum electrostatics models  
*Week 14:* Brownian dynamics simulations  
*Week 15:* Review  
**Final exam:** Wednesday, December 17, 8-11am, CARC 274

Lab exercise and homework schedule:

*Week 3:* Lab exercise #0: Introduction to MOE (tutorial from Chemical Computing Group)  
*Week 3:* Homework #1 due  
*Week 3-5:* Lab exercise #1: Force field dissection, energy minimization, and grid searches (using MOE)  
*Week 6:* Homework #2 due  
*Week 6-9:* Lab exercise #2: MD and MC simulation methods (using MOE)  
*Week 10:* Homework #3 due  
*Week 10-12:* Lab exercise #3: Protein electrostatics (using MOE)  
*Week 12:* Homework #4 due  
*Week 13-15:* Lab exercise #4: The DCM (using our code)  
*Week 15:* Homework #5 due

**Lab report format:** Inasmuch as possible, each lab report should follow standard journal article formats. Meaning, each lab report should have the following sections: (a) background, (b) methods/protocols, (c) results, (d) discussion, (e) conclusions, and (f) references. All appropriate figures should also be included. If desired, the results and discussion sections can be combined. When needed, appendices can also be added. Any standard reference format (in text citation and bibliography formatting) is acceptable so long as you are consistent throughout the report. With figures, I suspect that each lab report will be between 8 and 20 pages long.