BCHM 5984: Applications of Molecular Modeling
Fall 2009
MWF 9:05 – 9:55 AM, Litton-Reaves 1760

Instructors:

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Office Hours: By appointment

Course Website: http://scholar.vt.edu

Course Description

This course is designed for graduate students and senior-level undergraduate students who have a background in biological sciences and/or computational biology. The course will focus on practical and basic theoretical aspects of molecular modeling, such that the student can apply the techniques in their own research. Emphasis will be placed on understanding current literature and applying techniques to real-world problems.

Purpose of the Course

Due to the increasing accessibility of high-powered computing and molecular modeling software, computational techniques are becoming more widely used in biological research. This course is designed to teach students with an interest in molecular modeling the basic theories and common techniques that may be readily applied to their own research. Discussion will focus on protein modeling, but many of the techniques are easily applied to other molecules and systems of interest. Although a brief review of basic protein biochemistry will be provided, students are expected to have prior knowledge of protein structure and function.

Course Objectives

Upon completing the course, the student should be able to:

- Describe the basic theoretical aspects of molecular modeling techniques
- Evaluate the successes and limitations of molecular modeling
- Analyze the results of molecular modeling calculations
- Evaluate and discuss current literature related to molecular modeling
- Apply molecular modeling techniques to ongoing research

Course Materials

Reading assignments will come primarily from published scientific literature; references will be provided online through the Scholar site. Interested students may wish to purchase the following

text, although it contains more advanced topics that are beyond the scope of this course, and as such, it is not required.

A. Kukol, ed. Methods in Molecular Biology 443: Molecular Modeling of Proteins. Humana Press, 2008.

Evaluation

Grades will be assigned based on the following work:

- Homework (40%)
- Take-home midterm (20%)
- Paper presentation (10%)
- Final project (20%)
- Attendance and participation (10%)

Midterm
Essay-based take-home exam covering topics in protein structure determination and MD.

Final Project
Students will design a modeling project based on their own research (or something new), and they will approve it with the instructors. Their assignment will be to design several molecular modeling experiments they can perform to supplement the experimental aspects of their central research project. They will hand in a brief written summary in the form of an abbreviated grant proposal, and give a ~15 minute presentation on their project in the last week of class.

Attendance and Participation
Students will be expected to attend class regularly and participate in class discussions.

Tentative Lecture Schedule

Week	Dates	Lecture Topics
1	8/24 – 8/28	Introductory material and structural review, visualization
2	8/31 – 9/4	Protein structure-sequence relationships, homology modeling
3	9/7 – 9/11	Introduction to Molecular Mechanics and Molecular Dynamics
4	9/14 – 9/18	Molecular Dynamics algorithms
5	9/21 – 9/25	Molecular Dynamics applications, thermodynamics
6	9/28 – 10/2	Molecular Dynamics – pulling and advanced sampling techniques
7	10/5 – 10/9	Molecular Dynamics of complex systems *(no class Friday 10/9)*
8	10/12 – 10/16	Monte Carlo, protein domains, Normal Modes Analysis
9	10/19 – 10/23	Docking and *in silico* drug screening
10	10/26 – 10/30	Student paper presentations
11	11/2 – 11/6	Docking and *in silico* drug screening, QSAR
12	11/9 – 11/13	Macromolecular interactions
13	11/16 – 11/20	Quantum Mechanics
14	11/23 – 11/27	*(Thanksgiving break)*
15	11/30 – 12/4	Special topics and student presentations
16	12/7 – 12/9	Continue student presentations *(semester ends 12/9)*

Important Dates

31 Aug	HW 1 assigned
7 Sep	HW 2 assigned
11 Sep	HW 1 due
18 Sep	HW 2 due
21 Sep	HW 3 assigned
28 Sep	Papers for presentations assigned
2 Oct	HW 3 due
12 Oct	Midterm assigned
23 Oct	Midterm due
26-30 Oct	Student paper presentations
30 Oct	Topics for final projects due
9 Nov	HW 4 assigned
20 Nov	HW 4 due
2-9 Dec	Presentations of final projects

Honor Code

Students are expected to be familiar with and abide by the Virginia Tech Honor Code, which governs all academic work at this University, particularly with regard to plagiarism. This is especially important (and potentially problematic) when discussing material published in the literature. Care must be taken to discuss published papers in your own words. If sentences (or parts of sentences) are used verbatim, they should appear in quotations and cited. However, even a simple rewording of a published phrase (even if properly referenced) is inappropriate. The Virginia Tech Graduate School has prepared a detailed document dealing with the issue of plagiarism, which can be accessed online:

http://filebox.vt.edu/studentinfo/gradhonor/plagiarism.html

Accommodations

Any student who is in need of special accommodations should meet with the instructors as soon as possible to discuss any specific needs.