Biology 5476: Modeling Biomolecular Systems I Fall 2008

Class Meetings: Tuesday and Thursday, Lecture, 1:30-3:00, CCB Classroom
Friday, Laboratory, 2:-00-4:00, CCB Teaching Laboratory

Coursemaster: Jay Ponder (CCB 208, 362-4195, ponder@dasher.wustl.edu)

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Web Site: http://dasher.wustl.edu/bio5476/

Objectives: This course covers basic computer modeling and physical simulation techniques as applied to biomolecular structure and function. Laboratory sessions will expose the student to a variety of methods actively being used in current research.

Textsbook: There are no required textbooks. However, the books listed below may be useful for parts of the course, and are available from online booksellers:

Molecular Modeling: Principles and Applications, 2nd Ed., Leach, 2001
Understanding Molecular Simulation, 2nd Ed., Frenkel and Smit, 2002
Computer Simulation of Liquids, Allen and Tildesley, 1987
Simulating the Physical World, Berendsen, 2007
Introduction to Computational Chemistry, Jensen, 2007

Other Info: Bio 5476 is required by the DBBS Graduate Program in Computational Biology Knowledge of basic computer use, such as file editing and the ability to manipulate data via simple shell scripts is assumed. Some prior background in physical chemistry is recommended prior to enrollment, but is not required. Grades will be based on laboratory write-ups and a take-home final exam to be distributed the last week of the course.

Module 1: Empirical Force Fields & Quantum Mechanics

Aug 28	Molecular Mechanics Energy Functions	Ponder
Sep 2	Electrostatics and Polarization for MM	Ponder
Sep 4	Potential Surfaces and Optimization Methods	Ponder
Sep 5	Laboratory (Conformational Analysis)	Ponder
Sep 9	Basics of Molecular Orbital Theory	Ponder
Sep 11	User's Guide to QM Methods	Ponder
Sep 12	Laboratory (Protein Molecular Dynamics)	Ponder

Module 2: Monte Carlo & Molecular Dynamics Simulations

Sep 16	Monte Carlo Techniques	Ponder
Sep 18	Molecular Dynamics Techniques	Ponder
Sep 19	Laboratory (Computing Properties of Liquids)	Ponder
Sep 23	Computation of Properties from Simulation	Ponder
Sep 25	Path Methods for Navigating Potential Surfaces	Ponder
Sep 26	Laboratory (Trypsin/Benzamidine Complex)	Ponder

Module 3:	**Electrostatics & Solvation**	
Sep 30	Electrostatics & Solvation I	Baker
Oct 2	Eleectrostatics & Solvation II	Baker
Oct 3	Laboratory (Introduction to APBS)	Baker
Oct 7	Electrostatics & Solvation III	Baker
Oct 9	Electrostatics & Solvation IV	Baker
Oct 10	**No Class – DBBS Biochemistry/Biophysics Retreat**	
Oct 14	Electrostatics & Solvation V	Baker
Module 4:	**Free Energy Methods, Docking & Binding**	
Oct 16	Brownian Dynamics & Kinetics I	Sept
Oct 17	**No Class – Fall Break**	
Oct 21	Brownian Dynamics & Kinetics II	Sept
Oct 23	Free Energy Methods I	Sept
Oct 24	Laboratory	Sept
Oct 28	Free Energy Methods II	Sept
Oct 30	Docking & Binding	Sept
Oct 31	Laboratory	Sept
Module 5:	**Cheminformatics & Drug Discovery**	
Nov 4	QSAR and 3-D QSAR	Marshall
Nov 6	Pharmacophore Active Site Modeling	Marshall
Nov 7	Laboratory (3D QSAR)	Marshall
Nov 11	Structure-Based Drug Design	Marshall
Nov 13	Chemoinformatics	Marshall
Nov 14	Laboratory (Virtual Screening)	Marshall
Module 6:	**Homology Modeling, Structure Prediction & Design**	
Nov 18	Template-Based Modeling of Protein Structure	Marshall
Nov 20	Molecular Recognition: The Devil's in the Details!	Marshall
Nov 21	Laboratory (Ligand Refinement)	Marshall
Nov 25	Structure Prediction: Homology Modeling	Marshall
Nov 27	**No Class – Thanksgiving Break**	
Nov 28	**No Class – Thanksgiving Break**	
Dec 2	Structure Prediction: Threading Methods & *ab Initio*	Marshall
Dec 4	Structure Prediction: Design & Engineering	Marshall
Dec 5	Laboratory (Homology Modeling)	Marshall