

# QB110a: Numerical Modeling of Biological Systems

## Spring 2008

**Instructor:** Michael Hagan, Abelson 350; E-mail: [hagan@brandeis.edu](mailto:hagan@brandeis.edu)

**Office Hours:** 3-5PM, Monday, or by appointment.

**Meeting Time and Place:** Abelson 239, TF, 1:40 – 3:00.

### **Required course work:**

Homework will be handed out in class, usually one every two weeks. Expect fairly extensive reading assignments. A term paper will be due at the last day of classes. There will be no written exams, but you will be asked to prepare a short presentation on your term paper topic at the end of the semester.

### **Grading Procedure:**

50% – Homework. 30% – Term paper. 20% – Presentation.

### **Course Description:**

Currently biology is undergoing a revolution whereby quantitative experimentation is providing remarkable molecular details of the basic processes of life. In particular, recent advances in imaging methods enable the visualization of collective interactions, while single molecule techniques can probe specific molecular species. These experimental advances afford the perfect opportunity for synergy between theory and experiments. This course will present an introduction to numerical methods that are appropriate for modeling biological systems at various length and time scales. The aim will be to provide experimentalists and theorists with an appreciation of both the possibilities and limitations of these techniques. Our modeling efforts will range in resolution from examining enzyme motions at the atomistic level to organismal development at the cellular level to large-scale population dynamics. To develop and solve these models we will develop and use techniques such as molecular dynamics, Monte Carlo simulations, and numerical solutions of differential equations.

### **Course Outline**

- 1. Introduction and motivation for numerical modeling of biological systems**
- 2. Molecular interactions and dynamics**
  - The origin of forces and motions that make biology work
  - Newton's Laws and the equation of motion
- 3. Biomolecular structure and motions at the atomic level**
  - Classification of protein structures and the forces that stabilize them
  - Nucleic acid structures and hybridization reactions
  - Molecular dynamics simulations of biomolecules: unfolding a small protein

#### **4. Coarse graining: from atoms to cells**

- Equilibrium calculations and Boltzmann's formula
- Monte Carlo simulations: propagation of allosteric states in protein complexes
- Phase transitions in biology (e.g., DNA hybridization)

#### **5. Genetics and cell regulation**

- Numerical solution of reaction-diffusion equations
- Development of Drosophila

#### **6. Putting it all together--From atoms to cells to organisms**

- Virus dynamics: from assembly of individual proteins to epidemiology and population dynamics of infections

### **Suggested reading**

1. T. Schlick, Molecular modeling and simulation: an interdisciplinary guide, (Springer, 2002) ISBN: 038795404X
2. D. Frankel, B. Smit, Understanding Molecular Simulation: From Algorithms to Applications, (Academic Pr., 2001) ISBN: 0122673514
3. M. P. Allen and D. J. Tildesley, Computer Simulation of Liquids. (Oxford: Oxford University Press, 1987) ISBN: 0198553757. Reprint available: Oxford: Oxford University Press, 1989. ISBN: 0198556454.
4. K. Dill and S. Bromberg, Molecular Driving Forces, (Garland Science, 2003) ISBN 0815320515
5. B. Alberts et. al., Essential Cell Biology (Garland Science, 2003) ISBN 081533480X
6. P. Nelson, Biological Physics, (Freeman and Co., 2004) ISBN 0716743728.
7. V. Ambegaokar, Reasoning about luck, (Cambridge, 1996) ISBN 0521447372