



## QBIC MODELING AND SIMULATION WORKSHOP OUTLINE

### Course Description

The workshop will have three equally weighted components: Bioinformatics, Deterministic Modeling, and Statistical Modeling.

The Bioinformatics section will introduce computational tools and techniques for analyzing biomolecular (DNA, RNA, protein) sequences and structures, as well as quantitative data, arising from biological experiments. Students will learn about the major databases and repositories of bioinformatics information. No background in computer science is expected, but knowledge of introductory molecular biology and genetics will be assumed.

The Deterministic Modeling unit will provide the students with basic knowledge of MatLab programming techniques and numerical methods. They will learn about the modeling process and how to implement simple models in Matlab. Examples of empirical and mechanistic models in biology and physiology will be introduced, and students will solve them both analytically and numerically.

The Statistical Modeling component will teach the students how to use statistical models to represent the output of biological systems, use empirical distributions to model data generated from biological systems, and use Monte Carlo simulations to analyze complex biological systems.

### Syllabus

#### Weeks 1-2:

- Fundamentals of Biology
- Fundamentals of Statistics
- Fundamentals of Databases and the Internet
- Overview of Bioinformatics, Computational Biology, and Biotechnology
- Databases and Software Packages: GenBank, SWISSPROT, and BioPerl
- Sequence Alignment and Multiple Sequence Alignment: BLAST and CLUSTAL
- Phylogenetic Analysis: CLUSTALW, Phylip, and PAUP
- Molecular Structural Alignment, Analysis, and Visualization: DALI
- Microarray Data Analysis: CLUSTER, SAM, GeneCluster, and TreeView
- Detection tools for DNA Sequence Motifs: MEME and Consensus
- Tools for Comparative Genomics
- Next Generation Sequencing Techniques

#### Weeks 3-4:

- Basic MatLab Programming
- Modeling and the Modeling Process
- Basic Differential Calculus and Difference Equation Solutions using Matlab
- Numerical Techniques
- The Difference between Empirical and Mechanistic Models
- Equation Families, their uses, and how to apply them to Calculus and Biology

- The Connection between Mathematical Concepts and Basic Biological Processes
- Using Data to Optimize Biological Processes

Weeks 5-6:

- Review of Statistical Models  
(normal, lognormal, exponential, logistic, Weibull, and some extreme-value distributions)
- Techniques for Estimation of Model Parameters
- Testing for Model Fit
- Introduction to Empirical Distributions
- Converting Deterministic Biological Systems into Random Systems  
(to study output)
- Generation of Random Variables from Statistical Models  
(to study the effect of uncertainties on output)
- Building Simulation Models

### Grading

Grades are based on homework assignments, a semester project, and an exam (one per section, three total). The final grade will be an average of the three unit grades.

### Prerequisites

- BSC 1010 and BSC 1011 (General Biology I and II)
- An introductory course in Molecular Biology and Genetics
- MAC 2311 and MAC 2312 (Calculus I and II for Biology)
- STA 3111 and 3112 (Statistics I and II)

### Textbooks

#### Bioinformatics

Bioinformatics and Functional Genomics. Pevsner. ISBN: 0470085851

#### Deterministic Modeling

Introduction to MatLab 7. Etter, Kuncicky, and Moore. ISBN: 0131474928

Introduction to Modeling in Physiology and Medicine. Cobelli and Carson. ISBN: 0121602400

#### Statistical Modeling

Statistical Models in Engineering. Hahn and Shapiro. ISBN: 0471040357