

**CH 930 – Sampling Methods**  
**TTh 1100–1215**  
**158 Hunter Laboratory**

**Dr. Steven J. Stuart**  
**Office: 369 Hunter**  
**Phone: 656-5013**  
**Email: [ss@clemson.edu](mailto:ss@clemson.edu)**

## **Required Textbooks**

None. Handouts will be provided.

## **Other Reading**

### Classical methods

*Computer Simulation of Liquids*, M.P. Allen & D.J. Tildesley, Oxford 1987

The bible of classical simulation methods, with quite a bit of good statistical mechanics, but getting a bit dated.

*Molecular Modeling: Principles and Applications*, A. Leach, Prentice Hall 2001

Good survey of simulation methods, some statistical mechanics. Focused largely on biomolecular applications.

*Molecular Dynamics Simulation: Elementary Methods*, J.M. Haile

Good coverage of philosophical and statistical mechanics topics (ergodicity, sampling, accuracy, etc.). Useful descriptions of evaluating properties. Stops short of realistic potentials, ensembles, algorithms. Author is ex-Clemson faculty (chem. eng.).

### Statistical Mechanics

*Statistical Mechanics*, D.A. McQuarrie, Harper & Row 1976

The classic text on statistical mechanics.

### Math & Programming

*Numerical Recipes*, W. H. Press et al.

Excellent survey of computer implementation of basic mathematical algorithms.

Available in customized editions for your favorite language (F77, F90, C, ...)

*The Art of Computer Programming*, D.E. Knuth

Superb treatment of computer science (but not physical science) algorithms. The discussion of pseudorandom number generation is noteworthy.

## **Course Philosophy**

The emphasis of this course is on the tools (statistical, statistical mechanical, and modeling) that are needed to perform analysis of simple models in the physical sciences. Effort will be made to make the course equally relevant to computational scientists, who perform simulations exclusively, and experimental scientists, who use modeling only as a way of interpreting their experimental data.

The goals of this course is to enable the student to understand what statistical analysis is required for a given problem; to understand what sampling methods are appropriate for performing this

analysis; to understand how to perform this sampling and analysis; and to critically evaluate the results to understand how meaningful they are.

These goals will be accomplished through theoretical (textbook) knowledge of the statistics and statistical mechanics, through reading the literature, as well as through hands-on examples. These examples will sometimes come in the form of small projects, which will require some computer programming.

### **Attendance**

Attendance will not be taken, but is expected. Problems and projects will be assigned on an irregular schedule, and short problems will be due in the following class. Most material covered in lecture will not be duplicated in a textbook or handout, so poor attendance will be detrimental. If you miss class, you are responsible for obtaining the lecture notes and assignments from another student.

### **Late Policy**

Students are authorized to leave after 15 minutes if the professor or a substitute has not arrived.

### **Computers**

A computer account will be provided on a UNIX system for performing some of the assigned projects. If you have a UNIX account that you would rather use, you may do so. Some familiarity with both UNIX and some programming language (FORTRAN, C, C++, MATLAB, perl, python, etc) will be required to complete these projects. You need not have any prior experience with UNIX or programming, but should expect to gain some familiarity with them during this course.

### **Homework**

Homework problems will be assigned during class. These problems will be collected, and some will be graded, the following class period. If you miss a class, you are responsible for finding out whether any homework problems were assigned, and for making sure your problems from the previous class are submitted.

### **Projects**

There will be several larger homework assignments and projects. These may include a collection of homework problems, or a project in which the methods discussed in class will be implemented, applied, or assessed. Some programming will be required, but the early projects will not involve very much programming, and assistance will be provided for those with no programming background.

Some projects will be optional. These optional projects will provide “exam exemption points”. If you complete enough optional projects, you can be exempted from taking the midterm or final exams.

## **Group collaboration**

Group collaboration on homework assignments is not only allowed, but encouraged. Discussion of problems with other students is an excellent method for learning and reinforcing course material. However, all work to be submitted for a grade must be the product of the individual student. A simple rule of thumb is that you are allowed to discuss ideas and approaches, but you should not copy another student's work (including their programs), nor should you let another student copy your work.

## **Academic Integrity**

Official Clemson statement: "As members of the Clemson University community, we have inherited Thomas Green Clemson's vision of this institution as a 'high seminary of learning.' Fundamental to this vision is a mutual commitment to truthfulness, honor, and responsibility, without which we cannot earn the trust and respect of others. Furthermore, we recognize that academic dishonesty detracts from the value of a Clemson degree. Therefore, we shall not tolerate lying, cheating, or stealing in any form."

Class statement: Academic dishonesty of any sort – including cheating, plagiarism, illegal or unacknowledged assistance – is not tolerable in this class, or in the scientific or engineering professions. Such actions can ruin your career if you engage in them outside of the University. In this class they will be treated seriously, and can result in a failing grade for the course or expulsion from the University.

## **Exams**

There will be a midterm and a final exam. These exams can be exempted through completion of optional projects. Make-up exams will **not** be given without advance permission, a receipt from Redfern, or an official excuse from the registrar.

## **Grade Distribution**

Homework	20%
Projects	50%
Midterm	15%
Final exam	15%

## **Grade Scale**

90 - 100	A
80 - 89	B
70 - 79	C
60 - 69	D
0 - 59	F

## Syllabus

- Statistical Mechanics
  - ensembles
  - ensemble averages
  - thermodynamic properties
- Statistics
  - simple statistics
  - hypothesis testing
  - error estimation
  - correlation functions
- Sampling Concepts
  - weighted averages
  - unbiased sampling
  - biased sampling
  - ergodicity
- Sampling Algorithms
  - Monte Carlo, Markov processes
  - biased Monte Carlo
  - molecular dynamics
  - stochastic dynamics, Brownian motion
- Tools
  - minimization algorithms
  - pseudo-random number generators
  - temperature control
  - transition path methods
- Advanced Sampling Methods
  - kinetic Monte Carlo
  - parallel tempering
  - hybrid methods
  - Replica Exchange
  - accelerated dynamics
  - reaction path sampling