Computer Simulations in Physics

CAPS 424-02 Spring 2005

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Classes: TR 9:30 – 11 am Rooke Chemistry 017

Office Hours: TR 11 am – 12 pm, F 1 – 2 pm, and by appointment

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Text:

- H. Gould and J. Tobochnik, *An Introduction to Computer Simulation Methods*, 2nd edition, Addison-Wesley, Reading 1996.
- Any C++ reference. If you have no book yet I recommend: Jeri R. Hanly, *Essential C++ For Engineers and Scientists*, Addison-Wesley, Reading 2001. If you prefer a manual on the web, that is fine too.

Course Description: This course is about computer simulations in physics and related fields. During the last 30 years the computer has revolutionized the natural sciences and other disciplines such as economy and ecology. Computers have made it possible to study problems which are analytically not solvable. With computer simulations we can test models to find for example the reasons for traffic jams, stock market crashes, and the shapes of snowflakes. In these and many other examples, the model might be a simple rule for a single element, such as a a car, an investor, or a water molecule, which then gives rise to the complex behavior of the system as a whole. The computer takes care of applying the rules to a large number of elements.With computer simulations the models can be tested exactly contrary to experiments where for example impurities might play an additional rule. In nowadays science we use the interplay of theory, experiments and simulations.

Objectives: You will learn in this class how to write and run your own C++ programs and how to analyze the resulting data. We will start with an introduction to Unix and C++. For the remainder of the course you will learn about modeling via the examples listed in the course syllabus below and a project of your own choice.

Course Structure: This course will be a mixture of mini lectures, computer labs, and seminars (given by you!). As preparation for class you will get daily assignments such as reading assignments and small programs. You will work on class-related smaller projects which will be presented in class (see projects I – IV in syllabus). Since the course will be evolving based on your input, it will be essential that you come prepared to class.

Additionally, each of you will have your own project where you choose your subject, model, and literature, write your own program, and analyze the resulting data. You will present preliminary results in class. After "playing" with your program, you will present your final results in a public conference. You will be assisted with your project.

Grading: *There will be no exams and no final!* It is important that you work steadily on your project and the class preparations. Since this course is mainly in the form of in-class work and seminars, your participation is essential, and therefore attendance mandatory. If you must miss class (e.g. for a job interview), you *must* arrange with me *ahead of time* to make up the missed class. If this is not possible (e.g. last-minute emergencies), you must contact me immediately. Each unexcused missed class will result in 1/3 of a letter grade deduction from your final grade! Three unexcused missed classes result in an F. For any late *daily* assignment you will get **no** credit. For the projects I and II you will write 1-2 page long papers (for due dates see syllabus) and you will present your results in a 10 min long talk. On the projects III and IV you will work and present your results in class in groups of two. For the main project of your own choice you will write two papers. The first will be about the background of your subject and a precise description of the model. A complete description of your project, including model, program, data analysis and conclusions will be in your second paper. For any late paper you will get a 10% point reduction for each late calendar day (maximal reduction: 50%). We will make a pamphlet with the abstract for your final, public presentation. To maintain the right pace for your project note the deadlines given in the syllabus and marked with *.

Daily Assignments & Participation	25 %
Projects I & II:	
Papers	10 %
Talks	10 %
Projects IV & V:	10 %
Main Individual Project:	
Bibliography & Flow Diagram	5 %
First Paper	8 %
First Talk	8 %
Second Paper	8 %
Second Talk	8 %
Final Program	8 %

Course Syllabus

Date	Topic	Reading	Due Dates
Jan. 20	Introduction & Unix	Ch 1	
Jan. 25	Introduction to C++	App. B, C++ reference	
Jan. 27			
Feb. 1			
Feb. 3	Random Walks	§7.3 – 7.5, §12.1 – 12.3	
Feb. 8	Fractal Growth	Ch 14	Bibliography I*
Feb. 10			
Feb. 15			Bibliography II*
Feb. 17			Project I
Feb. 22	MD-Simulations & Chaos	§5.1 – 5.5, 5A Ch 6	
Feb. 24			
March 1			1. Paper: 1st Version*
March 3			Project II
March 8	Presentations of 1. Paper*		1. Paper: Final Version*
March 10			

Date	Topic	Reading	Due Dates
March 22 (?)	Ising Model	§11.7, §11.8	
March 24 (?)			Flow Chart*
March 29		§16.5, §16.6	
March 31		§17.1 – 17.6	
April 5	Project III		Program*
April 7	Many Particle Systems	§8.1 – 8.8	
April 12			
April 14			Results*
April 19	Project IV		2. Paper: 1st Version*
April 21	Traffic Flow	Handouts	
April 26			2. Paper: Final Version*
April 28	Presentations of 2. Paper*		
May 3			