CPS421/521 **Fall, 2002** MW 12:45-2:15 PM
Introduction to Computational Physics 132 Smith

Instructor:
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Office hours:
Tue 7:15 - 8:45 PM
Fri 2:30 - 5:00 PM
and by appointment

My Web page: http://www.cps.brockport.edu/~tuzun
Course Web page: Angel courseware system (http://angel.brockport.edu/angel)

Course materials

Nicholas J. Giordano, *Computational Physics*
Supplemental handouts, including material from the Web and other sources.

Course description

An introduction to computational methods used in real physics applications. Three of the most important differential equations in physics (Laplace, diffusion, and wave equations) will be discussed in the context of applications, along with several topics in classical mechanics and molecular simulation. The topics, in order of presentation, are

(1) Review of classical mechanics and conservation laws.
(2) Some celestial dynamics problems: detailed solution of two-body problem with 1/r interaction, simulation and analysis of trajectories, and many-body problems.
(3) Electric potentials and fields, Laplace's equation: some analytical solutions and some finite difference schemes for numerical solution.
(4) Wave motion: wave equation, superposition and wave packets, wave reflection and propagation, non-ideal media, numerical solution of wave and modified wave equations. In addition, normal coordinate analysis.
(5) Molecular dynamics simulation: basic methods for simulation and analysis/verification of simulation results, specification of initial conditions (temperature, pressure, and so on), constant temperature and/or pressure simulations, Langevin and Brownian dynamics, computation of transport properties such as viscosity, phase transitions, correlation functions and liquid structure.
(6) Diffusion and stochastic processes: diffusion equation and its derivation, simulation of diffusion processes, percolation, self-avoiding random walks, treatment of differential equations with diffusion terms (e.g., Schrodinger equation using quantum Monte Carlo).

Homework

Homework assignments will be given approximately once every week and a half, including one assignment due during finals week. These will include

- *Paper and pencil problems.*

- *Programming*---modification of code provided to you, or writing some simpler codes from scratch. Concepts to be developed include generality, robustness, accuracy, and efficiency, as well as bookkeeping issues.
- *Technical writing*---at least one question that requires a one- or two-paragraph answer.

You may work in Fortran 77 or 90, or in C/C++, whichever is comfortable. For those of you who know both Fortran and C/C++, I would suggest using both throughout the course. In order for me to be able to provide the best feedback possible, I will want to be able to follow and to reproduce your work (including all numerical results). Please see the Homework preparation link on my Web page for further details.

Computing environment

Each student will be given an account on the Computational Science department's Silicon Graphics Onyx 2 workstation. This computer has a UNIX operating environment; Fortran 77/90 and C/C++ compilers; and several graphical and general purpose packages such as MATLAB, MACSYMA, and xmgr.

Project for all class members

Instead of tests, there will be an approximately four-week project. The purpose of this project will be to explore in greater detail than a homework assignment a problem related to the class material. Fully detailed handouts will be provided later.

Additional responsibilities for CPS521 students

CPS521 students will have a significantly increased level of responsibility compared to CPS421 students. These additional responsibilities will include

- additional problems on each homework assignment.
- additional lecture material. Each major topic listed above will take approximately two to three weeks. CPS421 students will be expected to attend the first two-thirds of the lectures; CPS521 students will be expected all of them. The CPS521 lecture material will consist of more advanced material within the module, or additional topics. CPS421 students are welcome but not required to attend the CPS521 lectures.
- an additional four-week project given out just after the completion date for the first project. Fully detailed handouts will be provided later.

The Web

The course Web page will be updated frequently. In addition to being passed out in the classroom, assignments and handouts will be posted on the course Web page. Answer keys, class announcements, and so on will also be posted. No grades will be accessible from the Web.

Grading:

Projects: 40%, equally weighted.
Homework: 60%, equally weighted.

Late homework/projects will penalized 25% per day. In addition, you must complete (or at least attempt) every writing assignment in order to be able to receive an A or A- in the course.

Disability statement:

I would appreciate hearing from anyone who has a special need which may be the result of a disability. I am reasonably sure that we can work out whatever arrangements are necessary, whether special seating, testing, or other accommodation. See me after class or during office hours as soon as possible.