

Computational Physics I

(PHZ5156C, three credit hours) Spring 2013

Instructor: Dr. Inna Ponomareva, iponomar@cas.usf.edu, 974-7286

Course time: T&R 11:00 am – 12:15 pm

Classroom: ISA 4010

Instructor office hours: T&R 1:00 pm – 2:00 pm office ISA 5103, or by appointment.

Course objectives: To provide students with tools for using computers/supercomputers in research projects in physical, chemical and engineering sciences with a particular focus on nanoscience. All the course topics will be illustrated by practical examples in which the student will actively participate through modifying and executing these examples using computers/supercomputers in the classroom and performing homework. At the end of the course, the student will be expected to master sufficient number of tools to set up his/her own computational experiment. Particular emphasis will be given to use of internet resources for a quick access to the up-to-date information.

Requirements: Familiarity with some fundamental concepts of physics and chemistry (e.g., Newton's laws, interactions between atoms and molecules, etc...) is expected. No *a priori* computing skills are required. Computers accounts will be provided for both classwork and homework.

Course topics:

1. Linux/Unix operating systems (basic commands and services). Shell programming (script-writing).
2. Fortran 90 (writing, debugging, compiling simple codes), compiling larger codes utilizing makefile.
3. Parallel programming using MPI environment.
4. Computational techniques for research: different approaches to describe interatomic interactions (*ab initio*, tight-binding, empirical potentials), Monte Carlo and Molecular Dynamics, practical examples of using these techniques in computer codes.
5. Computations for nanoscience (the material of the previous topics will be used to solve a model computational nanoscience problem).

Homework: Homeworks (13 total) will be assigned for each topic of the course. Most of the homeworks require use of computer.

Grading: Homework 70%, Final quiz 30% (theory 10%, lab test 20%). Extra grade (up to 10 %) can be earned by incorporating the course material in the student's research projects. Overall grade:

$$G=0.7g_{\text{home}}(\text{average})+0.1g_{\text{theory}}+0.2g_{\text{lab test}}(+0.1g_{\text{extra}})$$

To assign letter grades, the following “straight scale” will be used : 85-100(A); 70-84(B); 55-69 (C); 40-54(D); 0-39(F).

Tentative Schedule and Examination Dates

Week Beginning	Topics (presentations), homework (HW) due dates
Jan 7	Linux, shell-scripting (pres1)
Jan 14	Introduction to Fortran90 (pres2), HW1 due Jan 17
Jan 21	Introduction to Fortran90 (pres2, pres3) HW2 due Jan 24
Jan 28	Introduction to Molecular Dynamics (pres4, pres5), HW3 due Jan 29, HW4 due Jan 31
Feb 4	Development and use of basic Molecular Dynamics code to simulate some materials properties (pres6), HW5 due Feb 7
Feb 11	
Feb 18	Introduction to parallel programming, parallelizing Molecular Dynamics code (pres7), HW6 due Feb 19
Feb 25	HW7 due Feb 26
Mar 4	Overview of computational techniques for materials research (pres8, pres9), parallel MD due Mar 5
Mar 11	Spring break
Mar 18	Ising model for ferromagnets (pres10), HW8, HW9 due Mar 19 (in the form of quiz)
Mar 25	
Apr 1	Computational Research Project (p1), HW10 due Apr 2
Apr 8	
Apr 15	Computational Research Project (p2), p1 due Apr 16
Apr 22	
Apr 29	FINAL, April 30th 10:00 am – noon, theory + lab test, p2 due Apr 30

NOTE

Students who anticipate being absent from exams due to a major religious observance must provide notice of the

date(s) and event(s) to the instructor, in writing, by the second class meeting. Notes and Tapes are not permitted for purposes of sale.

Any student with a disability is encouraged to meet with me privately during the first week of class to discuss accommodations. Each student must bring a current Memorandum of Accommodations from the Office of Student Disability Services (974-4309, SVC1133) which is prerequisite for receiving accommodations. Accommodated examinations through the Office of Student Disability Services require at least two weeks notice.