Computational Nanoscience
(PHYS 502V-032, one credit hour) Summer 2008

Instructor: Dr. Inna Ponomareva, Phys. ANNEX 293, 575-5596, iponoma@uark.edu
Course time: Monday and Thursday from 9:10 am to 10:30 am.
Classroom: PHYS0132/Lab118
Instructor office hours: by appointment, Monday-Friday (8:00 am – 5:00 pm).

Course objectives: To provide the student with the basic 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 and supercomputer 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 programing using MPI environment.
4. Overview of computational techniques for research: different approaches to describe interatomic interactions (*ab initio*, tight-binding, empirical potentials), Monte Carlo and Molecular Dynamics, practical example of using one of these techniques in a computer code.
5. Computations for nanoscience (the material of the previous topics will be used to solve a model computational nanoscience problem).
6. Final quiz.

Homework: Homeworks will be assigned for each topic of the course. Most of the homeworks require use of computer/supercomputer.

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:

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

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).