Course Syllabus COR502/CE621/MAE610/MTH668/PHY516 High Performance Computing II, Spring 2001 Tuesdays and Thursdays, 2:00-3:20, Natural Sciences Complex, room 222 Course web page: http://www.eng.bufalo.edu/Courses/ce621

- Instructor: Prof. Mark T. Swihart swihart@eng.buffalo.edu 907 Furnas Hall 645-2911 ext. 2205 Office Hours: Tuesdays and Thursdays 3:30-5:00 or call or e-mail ahead to meet at other times
- **Objectives:** This relatively new course, created through the cooperation of the Center for Computational Research and the Departments of Chemical Engineering, Mathematics, Physics, and Mechanical and Aerospace Engineering, introduces the fundamental ideas of scientific computing on high performance architectures. These computers, and the efficient algorithms developed for them, are enabling realistic simulations of many complex physical phenomena. Computational Science is becoming a third method of science, complementing theoretical and experimental research. A working knowledge of Computational Science is rapidly becoming an important tool for scientists and engineers working in a wide variety of areas. UB has made a significant investment in this area by setting up the CCR, currently one of the top 10 academic supercomputing centers in the US.

During this second semester of the course, we will concentrate on applications in computational science, including solving partial differential equations (including iterative solution of large sparse systems of linear equations), Monte Carlo methods, molecular dynamics simulations, and possibly computational quantum chemistry. The mix of these topics will depend, in large part, on the interests of the students participating in the course.

- **Prerequisites:** The sensible prerequisite for this course is High Performance Computing I, in which you presumably became familiar with architectures of modern high performance computing platforms, and developed passable skills in parallelizing codes using openMP on shared-memory platforms and MPI on distributed (or shared) memory platforms.
- Grade Basis: Exams: There will not be any exams in this course.

Project: Students will complete a substantial project on a topic of their own choosing. This will be due near the end of the semester, and will be presented in both oral form (to the class) and as a written report. The oral presentation will determine 20% of the course grade. The written report will determine 30% of the course grade. Oral presentations will be scheduled for the last few class periods of the semester. The final written report will be due on the last day of final exams (Thursday, May 10). No extensions beyond that date will be given.

Homework: Several homeworks will be assigned, and will determine 30% of the course grade. Working together on homework assignments is encouraged, but each

of you should submit a separate final homework solution, and should indicate, as appropriate, with whom you worked on the homework.

Colloquium Reviews: The CCR colloquium series seminars (approximately 6-8 of them) during the spring semester will be included as part of this course. They will generally be held during our course time, and in the room where we have class (NSC 222). At the next class meeting after each seminar, you should submit a 1-page (typewritten) summary and critique of the presentation. These seminar reviews will determine 20% of the course grade.

Text: There is no required text for this course. Some helpful links to web-based resources are included on the course web page. References for individual topics will be given as they are covered.