

CS6404: Modern Computational Science

Instructor: Dr. Alexey V. Onufriev, 2160C Torgersen Hall
Email: alexey@cs.vt.edu
Office Hours: 2 - 4 pm Wed

When and Where: Tue,Thu 3.30 pm MCB 318

Textbooks: See the web site

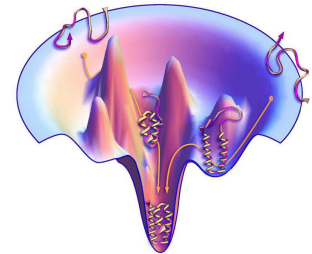
Course Notes: See the web site

Midterm: NONE

Final exam: Final project report, due date TBA

Course Website: TBA

Course purpose and structure This project-based course gives students hands-on experience with modern computationally intense research. Students will work in groups on realistic computational projects; they will be exposed to the entire life cycle of a research project, from initial brainstorming to final report. Each project will involve many aspects of modern scientific computing, such as choice of appropriate numerical methods and algorithms, choice of software, computational platform and visualization.



In the past, students from different disciplines and departments took the course (Physics, Bio, CS, GBCB), which made it a multi-disciplinary experience. Not everyone is expected to have the same background.

All projects will be computational, some will involve "supercomputing on the desk", that is GPU based computing on a user level (no GPU programming skills needed). Students will be able to do production quality research on par with what the best labs are now doing. A good number of projects will be biologically motivated (e.g. "protein folding on a supercomputer"), but not every single one. Specific projects will be announced in the first week of class, students will form teams and pick projects they like. One project per team.

Basic numerical methods relevant to each chosen projects, as well as useful unix tools will also be reviewed. The course will include instructor's lectures, student presentations (second half) and work on the projects. Access to real computational facilities will be provided.

Grades Final grade: 60 % will come from the project, and 40 % from the homework and student mini-presentations of original papers. The project grade will be based on the final report and student in-class presentations.