JOHNS HOPKINS
KRIEGER SCHOOL
*of* ARTS & SCIENCES

Syllabus
Simulating Nature: An Intro to Large Scale Computing
Physics & Astronomy 325.13 Intersession 2017

**Overview**

A single raindrop contains ~10^22 atoms but few problems with three or more particles can be solved by hand. High performance computing gives researchers the ability to simulate billions of atoms and numerically solve otherwise intractable problems. This course gives students an interactive introduction to using supercomputers to simulate matter at the atomic scale and analyze the resulting behavior with Python. Students will learn the basic skills of a computational scientist and use them to explore applications in engineering, biology, and physics. No prior knowledge of programming necessary.

**Instructors**


Thomas O'Connor
toconnor@jhu.edu
329 Bloomberg
Office hours TBD

Joel Clemmer
jclemme3@jhu.edu
329 Bloomberg
Office hours TBD


**Lectures**

Lectures will meet from 10:00-11:45am on Monday, Tuesday, and Thursday in room TBD. The course will meet beginning the week of Monday 1/9/2017 until the week of 1/27/2017.

**Resources**

During the course students will receive access to a high performance computing cluster. In order to access the cluster, students will need to bring a laptop to class. During the course students will learn how to use a variety of free software possibly including:

Python (https://www.python.org/)
Cyberduck (https://cyberduck.io/?l=en)
LAMMPS (http://lammps.sandia.gov/)
Ovito (http://www.ovito.org/)

**Assignments**

Following each lecture, there will be computational assignments. These assignments will consist of simulating a physical system, analyzing the data, and understanding the physics involved. There will be time dedicated in-class to work on these assignments with instructor guidance. Assignments may also have a short component outside of class.

Depending on how fast course material is covered, there may be a small course project. The project would have students design and run their own simulation and give a short presentation on the results. Time in-class would be allocated to work on the project.

**Anticipated Course Schedule**

| Date | Topic |
|---|---|
| 1/9/2016 | Overview of course and introduction to Unix |
| 1/10/2016 | Introduction to python and data analysis |
| 1/12/2016 | Molecular dynamics (MD) and visualizing atomistic data |
| 1/16/2016 | Thermodynamic ensembles and LAMMPS |
| 1/17/2016 | Identifying phases and melting solids |
| 1/19/2016 | Nonequilibrium systems and salt shakers |
| 1/23/2016 | Stress strain relations and sheared solids |
| 1/24/2016 | Polymers and liquid crystal transitions |
| 1/26/2016 | Timescales and shock dynamics |
| Time permitting | Non-MD simulations: bird flocking, surface growth |

**Ethics**

The strength of the university depends on academic and personal integrity. In this course, you must be honest and truthful. Ethical violations include cheating on exams, plagiarism, reuse of assignments, improper use of the Internet and electronic devices, unauthorized collaboration, alteration of graded assignments, forgery and falsification, lying, facilitating academic dishonesty, and unfair competition. As noted above, collaboration on homework sets is encouraged. However, you should attempt problems independently before collaborating and must write up your homework independently.

Report any violations you witness to the instructor. You may consult the associate dean of students and/or the chairman of the Ethics Board beforehand. See the guide on "Academic Ethics for Undergraduates" and the Ethics Board web site (http://ethics.jhu.edu/) or http://www.advising.jhu.edu/ethics.html for more information.

**Students with Disabilities**

Any student with a disability who may need accommodations in this class must obtain an accommodation letter from Student Disability Services, 385 Garland, (410) 516-4720, studentdisabilityservices@jhu.