

Foundations of Programming and Software Engineering



Daily Schedule

09:00 AM - 10:30 AM PT Instruction

10:30 AM - 10:40 AM PT Break
10:40 AM - 12:00 PM PT Instruction

12:00 PM – 01:00 PM PT Break

1:00 PM – 04:00 PM PT Zoom Group Work

-- Continue working on assignments if necessary -

- Dr. Pritchard and Dr. Nash are available for office hours from 4:00 PM to 6:00 PM PT
- Incorporate daily group pull requests by next class session (we'll explain what this means!)





Your Instructors



Dr. Jessica Nash



Dr. Benjamin Pritchard





What will you learn?

Expectations – At the start of the course, we expect that you understand Python syntax.

By the end of this course, you will be able to answer these questions:

- Broadly, what is Monte Carlo simulation?
- How can I use Monte Carlo simulation to predict the properties of a chemical system?
- What is the Python Standard Library?
- How can I use git to keep a record of my project?
- How can I use GitHub to share code and collaborate on projects?
- What is one of defining features of the array in the library NumPy?
- How can I make visualizations in python?
- What is the difference between an interpreted and a compiled programming language?
- What is the syntax of the C++ programming language?





What is our goal?

First and foremost – our goal is to learn! ☺

In this course, we will be implementing a Monte Carlo simulation of a Lennard Jones fluid.

- 1. Implementation with the Python Standard Library
- 2. Implementation with NumPy
- 3. Implementation in C++

We will compare our simulation to benchmarks computed by the National Institutes of Standards and Technology (NIST).

We will also compare simulation results to experimental data reported by NIST – how accurate are our simulations?

We will compare performance of different implementations of our code. Which is fastest? Python, NumPy, or C++ implementation?





Assignments

Individual Assignments – Individual programming challenges. To be completed on your own (4 total).

Blog Posts – Each group will have a blog where you have to write reflections each day. You should rotate in your group who writes the blog post, but the other group members should review and approve the post.

Group Assignments – Daily group programming challenges. You should complete one task and review the work of one of your groupmates each day. Submission and review will be on central team repository.

Presentation – On the last day of the course, each group should wrap up their project and present to the class (15 minutes per group).





Course Communication

bCourses – Your homepage for the course. Has links to text lessons and assignments.

Piazza – Class-wide discussions and announcements. Instructors can be contacted here.

GitHub – Assignments will be put here. Will also be used for peer code review and discussion.

Slack – Can be used for discussion with your group or classmates. Can be used for social discussion as well!





Class Code of Conduct

Our Pledge

In the interest of fostering an open and welcoming environment, we as students and instructors pledge to making participation in this course and our community a harassment-free experience for everyone, regardless of age, body size, disability, ethnicity, gender identity and expression, level of experience, nationality, personal appearance, race, religion, or sexual identity and orientation.





Class Code of Conduct

Our Standards

Examples of behavior that contributes to creating a positive environment include:

- Using welcoming and inclusive language
- Being respectful of differing viewpoints and experiences
- Gracefully accepting constructive criticism
- Focusing on what is best for the community
- Showing empathy towards other community members

Examples of unacceptable behavior by participants include:

- The use of sexualized language or imagery and unwelcome sexual attention or advances
- Trolling, insulting/derogatory comments, and personal or political attacks
- Public or private harassment
- Publishing others' private information, such as a physical or electronic address, without explicit permission
- Other conduct which could reasonably be considered inappropriate in a professional setting



