COMP 260

Special Topics: Scientific Computing

Syllabus

COMP260-01, Spring 2017
MW 10:50-12:10
Exley 141

Prof. Kelly M. Thayer
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Office hours: M 8:30-10:40, T 10:10-11:15, W 9:40-10:40 & 5:00-6:00
Please send an email request for appointments at other times.

GENERAL INFORMATION

Text: Primary literature from journals and excerpts from various texts will be used. All required materials are either freely available or will be posted on Moodle for download. Please refer to Moodle and the Course Calendar for specific readings by week.

Course Description: Welcome to Scientific Computing. This course will introduce students from various disciplines to computing as applied to scientific problems. The course aims to both provide solid background information through lectures and develop a strong computational skill set through active learning. Students from across the sciences will collaborate interactively in a small group to write computer programs to solve problems drawn from chemistry, physics, biology, and bioinformatics. Topics covered will include simulation techniques, analysis of trajectories, clustering, probabilistic modeling, networks, population dynamics, and high performance computing. Throughout the semester students will develop and implement an original research project using skills from the course to investigate a topic of their choice.

Moodle Web Site: A course web site has been established through Moodle, and it will continue to be developed throughout the semester. This serves as a central location where assignments, handouts, and announcements will be posted.
GRADING

Your course grade is comprised of several components (described below) as follows:

- 25% Seminar Discussion Participation
- 15% Literature Article Presentations
- 20% Laboratory Exercises
- 10% Lab Portfolio
- 30% Final Project

Seminar Discussions: Monday class meetings will follow a seminar discussion format based around the readings for the topic of the week. The readings will be posted in advance on the Moodle page. Discussion questions to focus and guide your reading will also be provided. The Seminar Discussion Participation grade will be based upon your participation in the seminar discussions; students are expected to have completed the readings and to engage in scholarly discussion of the material with a focus on the provided questions. Students are invited to participate by raising questions of their own to discuss, and by providing discipline specific perspective on the topic. The course is designed for the confluence of ideas from various perspectives, so being actively engaged and willing to discuss your experiences related to the topic will benefit all.

Literature Article Presentations: Students will sign up for leading ~10-15 minute discussions on journal articles from the primary literature exemplifying an application of the methods discussed in the course. Number of presentations will be based on registration totals. They will generally occur on Mondays and follow one week after the corresponding seminar discussion. The content should focus on how the method has been implemented in current research and what benefits computing has provided to the researchers.

Laboratory Exercises: During the Wednesday meetings students will engage in hands-on activities in which they will acquire practical experience with scientific computing. Some exercises will entail python coding of algorithms, whereas others will be based on guided tutorials. Students will interact with their classmates from various backgrounds, working together to solve problems. Students will be graded on active engagement in the lab exercises. While the completed exercises will not be collected each week, students are strongly encouraged to do so. The final version will be collected in the Lab Portfolio.

Lab Portfolio: While lab exercises should be able to be completed or nearly completed during class time, the finalized versions should be compiled by the end of the semester. The code should be working and well documented, and the tutorials should be completed. This work may represent a group effort and/or a group effort plus your own work, but should be compiled individually. It is due at the conclusion of the semester.
**Final Project:** In lieu of a final examination, the course will culminate in the completion of a final research project. It will be an opportunity for students to showcase your ability to apply computer science to answer scientific questions. It will involve applying the skills learned during the laboratory component to answer three questions of scientific interest. Students will be free to develop your own research topic with the professor’s guidance, and will receive mentorship at various checkpoints throughout the semester, including a project proposal worksheet in which a project topic is proposed, and preliminary results in which 2/3 of the anticipated results will have been attempted. Please refer to the course calendar for the dates. The project will entail writing code and/or performing calculations, and writing up the results into a report following the scientific journal format. Three questions should be addressed, and at least two distinct methods should be used for the project. Ideally it should involve both python coding and using Wesleyan’s high performance computing cluster. There will be a brief presentation during the last week of classes in which the preliminary results of each student will be shared with the class. A detailed guide sheet will be provided to delineate the details of the content of the presentation and project report. The written report including finalized results will be due during the final exam week on a date in accord with the guidelines set forth by the registrar; the date and time will be announced when the registrar announces this semester’s exam schedule.

**COURSE POLICIES**

**Attendance:** Students are expected to arrive to class promptly. If not feeling well, inform the instructor prior to the class meeting in as timely a fashion as possible and make up work will be considered on a case by case basis. In the event of serious illness or emergency, please contact your class dean, who will in turn inform all instructors that you will be taking an excused absence.

**Late Projects:** The final project must be turned in on the due date to ensure that it will be able to be graded prior to the due date of final grades to the registrar’s office. Please plan to work on it throughout the semester. Late projects will not be accepted.

**Academic Honesty:** Copying all or part of the work of others and claiming it as yours or allowing someone else to copy your work and claim it as theirs is a violation of the Honor Code. Apparent infractions will be reported to the Honor Board in accordance with the policies set forth in the Student Handbook ([http://www.wesleyan.edu/studentaffairs/studenthandbook/20162017StudentHandbook.pdf](http://www.wesleyan.edu/studentaffairs/studenthandbook/20162017StudentHandbook.pdf)).

**Religious Holiday Observance:** The instructors support Wesleyan’s policy with regard to absence due to religious holidays. If you have a conflict due to observance of a religious holiday, please alert the instructor in advance so that a plan for makeup can be arranged.
Questions regarding religious holidays may be directed to the University chaplains and/or to the Class Deans.

**Academic Accommodations:** The instructor is committed to supporting the Americans with Disabilities Act of 1990 and carrying out the mission of Disabilities Resources to create an accessible and inclusive learning environment where disability is recognized as an aspect of diversity. Students with disabilities are entitled to request reasonable accommodations and/or modifications in their classes at the beginning of each semester by filling out the Academic Accommodation Request Form (link found here: [http://www.wesleyan.edu/studentaffairs/disabilities/Student/Academic%20Accommodations.html](http://www.wesleyan.edu/studentaffairs/disabilities/Student/Academic%20Accommodations.html)) and meeting with the dean. The dean, in conjunction with the student, will prepare a letter for the instructors indicating the appropriate accommodations for the course. Students are encouraged to come at office hours or for an appointment to discuss their accommodation letters.