# Syllabus: BIOSC 1640: Computational Biology Research

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# Contents


**1 General Information** **3**
- 1.1 Instructor . . . 3
- 1.2 Class Description . . . 3
- 1.3 Lecture Schedule . . . 3

**2 Assignments** **4**
- 2.1 Software (37% of Final Grade) . . . 4
- 2.2 Participation (10% of Final Grade) . . . 5
- 2.3 Written Research Report (38% of Final Grade) . . . 5
  - 2.3.1 Description . . . 5
  - 2.3.2 Introduction Rough Draft (8% of the Final Grade) . . . 5
  - 2.3.3 Materials-and-Methods Rough Drafts (8% of the Final Grade) . . . 6
  - 2.3.4 Results-and-Discussion Rough Drafts (8% of the Final Grade) . . . 6
  - 2.3.5 Peer Review Assignments (6% of the Final Grade) . . . 7
  - 2.3.6 Final Research Report (8% of the Final Grade) . . . 7
- 2.4 Midterm Group Presentation Describing Progress (5% of the Final Grade) . . . 7
- 2.5 Final Group Presentation Describing the Project (10% of the Final Grade) . . . 8

**3 Grading Policies** **8**
- 3.1 Final Grade . . . 8
- 3.2 Withdrawal Policy . . . 8
- 3.3 G Grades . . . 8

**4 Course Materials** **9**
- 4.1 Required Materials . . . 9
- 4.2 Course Website . . . 9

**5 Additional Information and Resources** **9**
- 5.1 Acknowledgement . . . 9
- 5.2 Classroom Recording . . . 9
- 5.3 Academic Integrity . . . 9
- 5.4 Disability Resources . . . 9
- 5.5 E-Mail Communication . . . 10

# 1 General Information

## 1.1 Instructor

**Instructor**: Jacob D. Durrant
**Email**: durrantj@pitt.edu

## 1.2 Class Description

Students will use computational-biology methods to address an authentic research question. The course goal is to further expose students to computer programming and some of the basic principles of computational structural biology. Students will learn through lectures taught by Dr. Durrant and a hands-on group project. The class project will allow students to apply the relevant tools and to demonstrate their acquired knowledge. Grades will be based on codebase functionality and style, a written report, and midterm/final presentations.

Prior experience programming in Python is essential. If your case is unusual, contact me about a possible exception.

## 1.3 Lecture Schedule

Lectures and group coding sessions are on Fridays, from 1:00 to 3:30 PM, in A214 Langley Hall. The lecture schedule below (Table 1) may change based on the needs/interests/pace of the class. Always consult GitHub for an up-to-date syllabus.

**Table 1:** Lecture schedule (subject to change).

| Date | Topic |
|---|---|
| 1-10-20 | Review syllabus and group project. Visual Studio Code. Git. |
| 1-17-20 | Python basics. |
| 1-24-20 | Advanced Python. |
| 1-31-20 | Third-party Python libraries. |
| 2-7-20 | TBA |
| 2-14-20 | TBA |
| 2-21-20 | TBA |
| 2-28-20 | TBA |
| 3-6-20 | TBA |
| 3-13-20 | Spring break. |
| 3-20-20 | Extended spring break. |
| 3-27-20 | TBA |
| 4-3-20 | TBA |
| 4-10-20 | TBA |
| 4-17-20 | Final presentations. |

Lectures are unlikely to take the full 2.5 hours, and some class periods may not have lectures. Once the lecture finishes, students should get together with their groups and work on their programming and writing projects.

1. Start by discussing what you accomplished this past week. What went well? What could go better?
2. Make a detailed plan describing what you will accomplish next week, dividing the tasks among your group members.
3. Present your accomplishments and plan to the class (five minutes), get feedback.

4. Begin working on the tasks together. You may need to meet outside of class as well to finish the week's work.

I will also be available during this time should you have any questions about the project goals.

# 2 Assignments

Scores on coding functionality, participation, written reports, and presentations will determine final grades. If circumstances require us to reschedule any assignment due dates (Table 2), I will update the syllabus on GitHub.

**Table 2:** Assignment schedule (subject to change).

| Due Date | Description | Group or Individual Assignment? |
|---|---|---|
| 1-17-20 | Pseudocode | Group |
| 1-24-20 | Introduction Section | Group |
| 1-24-20 | Project Schedule | Group |
| 2-7-20 | Introduction Peer Review | Individual |
| 2-21-20 | Materials and Methods Section | Group |
| 2-28-20 | Midterm Presentation | Group |
| 3-6-20 | Materials and Methods Peer Review | Individual |
| 3-31-20 | Results and Discussion Section | Group |
| 4-3-20 | Results and Discussion Peer Review | Individual |
| 4-10-20 | Final Paper | Group |
| 4-17-20 | Final Presentation | Group |

## 2.1 Software (37% of Final Grade)

Part of your grade will be based on whether your program works. Students are responsible for breaking their programming tasks into smaller steps and for pacing their progress to ensure timely completion. We will discuss our code in class, so students should always bring a laptop computer. **If you don't have a laptop, speak with me during the first week of class.** If necessary, you might consider checking out a laptop from Hillman Library.

Your grade will also be based on how rigorously you test your software. I recommend creating test data so you can always make sure your program is working, even with regular updates. Documentation is also critical. You should create detailed instructions re. how to run your software. The README.md file should be in Markdown format.

As a capstone course, this class will require you to be self motivated and independent, as if you were a professional software engineer. You might need to learn new programming techniques, Python libraries, etc. Before asking for programming help, be sure to thoroughly research the question on your own. Learning how to independently overcome programming hurdles is as much a part of this course's objectives as the research project itself.

Groups of roughly six students will work together on coding projects. The overall goal of these projects is to improve my lab's ProteinVR program for molecular visualization. Each group will be assigned one of two projects:

1. **Project 1**. A program for calculating the smallest sphere that encompasses a set of three-dimensional points. Use that program to calculate spheres that encompass different sets of protein-model atoms (e.g., entire models, chains, and residues). Use the residue-encompassing spheres to intelligently position text labels in 3D space.
2. **Project 2**. A program for interpolating between multiple protein conformations. Not just a linear interpolation, but something smoother. Should not use the SciPy Python package (but NumPy is fine).

If necessary, I may expand the scope of these projects to accommodate group progress.

## 2.2 Participation (10% of Final Grade)

Attendance and participation are critical. Students who answer questions in class should send me a brief email **on the same day** explaining their participation. I may not accept explanations sent later than that. I will keep these emails and will draw on them when assigning participation points. The goal is to encourage students to pay attention during class. Evidence of inattention will adversely affect the participation grade, but incorrect answers or comments will not.

## 2.3 Written Research Report (38% of Final Grade)

### 2.3.1 Description

**Style..** The written research report should describe your coding project in detail. It should be divided into three sections: *Introduction*, *Materials and Methods*, and *Results and Discussion* (see below). You may further divide these sections into smaller sub-sections (with additional sub-headings) to clarify your intended organization. The report should be written in a scientific style. Consider using the Hemingway Editor to cut down on wordiness.

All sections of the research project should include references from the scientific literature that support your assertions. Internet web pages such as Wikipedia do not count as support. Also, citing a paper does not mean you are free to quote from it directly. To avoid plagiarism, be sure to use your own words. You may use any standard reference style (e.g., Vancouver, Harvard, APA, MLA, etc.).

The document should be single spaced, 12-point Times New Roman font, with 1 inch margins on all sides. Students may use charts, graphs, and illustrations is help explain complex topics. The lengths of each section are given below.

**Submitting sections for evaluation..** Each project section is due at the beginning of class (Table 2). I may not accept sections turned in after that time unless you provide a documented reason that is outside of your control. I also reserve the right to deduct points for late submissions. Don't forget to include the FULL names of all group members beneath the project title. Every time you email me a section of the report, start the subject line with "BIOSC 1640:".

Students must submit assignments in Microsoft Word (DOC or DOCX) or PDF formats. Documents written using other word processors should be converted to one of the above formats before sending them to me. Documents sent in other formats may be returned. Students who fail to use an appropriate format may be substantially penalized.

**All group members should participate equally..** Research-project submissions should include a separate, confidential email with a "percent effort" evaluation. It should include a list of all group members and your personal assessment of the percent effort (meaning writing + code) that each contributed to the assignment. I will take the information in these confidential emails into account when grading the group assignments. If the group feels that one of its members is not contributing to the project, please talk to me as soon as possible. Every student must contribute substantially to every section of the document. It is not acceptable, for example, for one group member to write the *Background* section, and another to write the *Results and Discussion*.

### 2.3.2 Introduction Rough Draft (8% of the Final Grade)

The *Introduction* section should be one to two pages long (single spaced). See this like the *Introduction* of a scientific publication. Start general and gradually get more specific. Be sure to answer these questions:

- What is the biological question at hand?

- Why is that question important?
- What existing methods/programs exist for answering this question? Why are they inadequate?
- Briefly, what is our solution? How is it better than the existing tools?
- Send me a separate, confidential email with a "percent effort" evaluation. It should include a list of all group members and your personal assessment of the percent effort (meaning writing + code) that each contributed to the assignment.

This assignment will be due on 1-24-20, pending any changes to the syllabus (Table 2). It is the students' responsability to consult the latest version of the syllabus (posted on GitHub) to verify all due dates.

#### 2.3.3 Materials-and-Methods Rough Drafts (8% of the Final Grade)

The *Materials and Methods* section should be one to two pages (single spaced). This section should read like the *Material and Methods* section of a scientific manuscript. Include the following information:

- What are the general details of your approach? What programming language, libraries, and established algorithms (if any) did you use?
- How does your the program work? A step-by-step description of each part of the algorithm (but not a line-by-line description).
- For each step, be sure to mention the required input(s) (variables).
- For each step, also mention the output(s) (return types).
- Send me a separate, confidential email with a "percent effort" evaluation. It should include a list of all group members and your personal assessment of the percent effort (meaning writing + code) that each contributed to the assignment.

This assignment will be due on 2-21-20, pending any changes to the syllabus (Table 2). It is the students' responsability to consult the latest version of the syllabus (posted on GitHub) to verify all due dates.

#### 2.3.4 Results-and-Discussion Rough Drafts (8% of the Final Grade)

The *Results and Discussion* section should read like the *Results and Discussion* section of a scientific manuscript.

- Put together a test data set.
- Apply your code to that test set.
- Describe the results to show that your program works.
- Send me a separate, confidential email with a "percent effort" evaluation. It should include a list of all group members and your personal assessment of the percent effort (meaning writing + code) that each contributed to the assignment.

This assignment will be due on 3-31-20, pending any changes to the syllabus (Table 2). It is the students' responsability to consult the latest version of the syllabus (posted on GitHub) to verify all due dates.

#### 2.3.5 Peer Review Assignments (6% of the Final Grade)

Although the sections themselves should be written as a group, each group member will independently and individually edit his or her own copy of the other group's sections. Rather than combine your edits with those of your fellow group members, turn in your own copy separately with only your own edits. For all peer-review assignments, students will be graded individually rather than as groups.

Edit for brevity, clarity, formatting, references, grammar, tone, etc. Be thorough in your edits. This assignment requires more than just reading over the report and saying "it looks good." The goal is to develop scientific-editing skills, which are critical in many bioscience jobs.

**Track all your changes** so I can review them. Tracking changes will also help the original authors better understand how to improve. Add a new section entitled "Reviewer" to the document you're editing. Place your FULL name in this section. Creating this separate section is critical so I can distinguish between those who originally wrote the document and the person who edited it.

Assuming there are no changes to the syllabus (Table 2), the three peer-review due dates are:

- Introduction section: 2-7-20
- Materials and Methods section: 3-6-20
- Results and Discussion section: 4-3-20

#### 2.3.6 Final Research Report (8% of the Final Grade)

After implementing the edits you receive from me and/or your peers, your group should combine the latest versions of your *Background*, *Materials-and-Methods*, and *Result-and-Discussion* sections into a single document. Remove the paragraphs describing the contributions of each group member. The document should be entirely up-to-date. The final report should also include a "Works Cited" section with full references.

This assignment will be due on 4-10-20, pending any changes to the syllabus (Table 2). It is the students' responsability to consult the latest version of the syllabus (posted on GitHub) to verify all due dates.

### 2.4 Midterm Group Presentation Describing Progress (5% of the Final Grade)

The midterm presentation should last ten to fifteen minutes. All group members should participate. Be sure to email me a copy of your slides afterwards. The presentation slides should answer these questions:

1. What have you accomplished so far?
2. What is the current status of your project?
3. Has anything changed in your approach since your initial plan?
4. What about your software-development process is working well?
5. What isn't working well?
6. How have you divided the work among all members of your group?
7. Is the project currently on track?
8. What are your specific plans to finish the project on time?
9. What course corrections are needed to meet your end goal?

This assignment will be due on 2-28-20, pending any changes to the syllabus (Table 2). It is the students' responsability to consult the latest version of the syllabus (posted on GitHub) to verify all due dates.

### 2.5 Final Group Presentation Describing the Project (10% of the Final Grade)

The final presentation should last about fifteen minutes. All group members should participate. The presentation slides should cover the same material covered in your final written project, with a similar organization. Be sure to answer the same questions in the oral presentation that I asked you to answer in the final written report. See the latest version of the syllabus if you need clarification.

The final presentation should also include:

- A "Works Cited" slide with full references
- A demo of your software
- A description of features and technical decisions

A five-minute question-and-answer session will follow each presentation. Be sure to email me a copy of your slides afterwards.

This assignment will be due on 4-17-20, pending any changes to the syllabus (Table 2). It is the students' responsability to consult the latest version of the syllabus (posted on GitHub) to verify all due dates.

## 3 Grading Policies

### 3.1 Final Grade

I will calculate letter grades according to the following scale: A (≥94%), A- (≥90%), B+ (≥86%), B (≥83%), B- (≥80%), C+ (≥76%), C (≥73%), C- (≥70%), D+ (≥66%), D (≥63%), D- (≥60%), F (<60%). I reserve the right to curve the grading scheme to benefit the class if I think it's appropriate. I also reserve the right to provide extra-credit points.

### 3.2 Withdrawal Policy

If you are unable to stay current with the material, regardless of the reason, consider withdrawing from the course. Please consult the official academic calendar to learn when the add/drop period ends and when the monitored withdrawal form must be submitted to the Dean's Office.

### 3.3 G Grades

In some rare cases, extenuating personal circumstances arising after the withdrawal deadline may prevent a student from finishing the course. Per SAS guidelines, if such a student has been attending the course and making regular progress, he or she may petition for a G grade (University of Pittsburgh Undergraduate Bulletin, 1999-2002, p.29). If you find yourself in this situation, send me a request in writing that documents your reason(s) for the grade-change request. You will have to complete the course work before the G grade can be removed.

# 4 Course Materials

## 4.1 Required Materials

This course does not require a textbook. I will post links to online resources, articles from the scientific literature, etc., on GitHub to support what we discuss in class.

## 4.2 Course Website

Course materials, an up-to-date syllabus, and a discussion board will be available through GitHub.

# 5 Additional Information and Resources

## 5.1 Acknowledgement

Students agree that I (Jacob Durrant) am free to incorporate the code created in this class into published software, without restrictions. I may similarly incorporate text from the written reports into any future publication. Students agree that I have exclusive claim to any relevant intellectual property rights. Students also agree that I will be solely responsible for making all decisions related to authorship and acknowledgement in future scientific publications. Such decisions will be made based on my assessment of the strengths of student contributions, as well as other factors such as whether students respond to future queries.

## 5.2 Classroom Recording

Students may not record classroom lectures, discussions, and/or activities without my written permission. Any recordings I approve must only be used by the authorized student, for their own private use.

## 5.3 Academic Integrity

Cheating/plagiarism will not be tolerated. Students suspected of violating the University of Pittsburgh Policy on Academic Integrity will be required to participate in the outlined procedural process as initiated by the instructor. A minimum sanction of a zero score for the homework, exam, or presentation will be imposed.

Students agree that by taking this course all required papers may be subject to plagiarism detection using iThenticate or some other automated system. All submitted papers may be included as source documents in the iThenticate (or other) reference database for the purpose of detecting plagiarism of such papers.

## 5.4 Disability Resources

If you have a disability for which you are, or may be, requesting an accommodation, you are encouraged to contact both the instructor for this course and the Office of Disability Resources and Services, 140 William Pitt Union, 412-648-7890/412-624-3346 (Fax), as early as possible in the term. Disability Resources and Services will verify your disability and determine reasonable accommodations for this course.

## 5.5 E-Mail Communication

Each student is issued a University e-mail address (username@pitt.edu) upon admittance. This e-mail address may be used by the University for official communication with students. Students are expected to read e-mail sent to this account on a regular basis. Failure to read and react to University communications in a timely manner does not absolve the student from knowing and complying with the content of the communications. The University provides an e-mail forwarding service that allows students to read their e-mail via other service providers (e.g., Hotmail, AOL, Yahoo). Students that choose to forward their e-mail from their pitt.edu address to another address do so at their own risk. If e-mail is lost as a result of forwarding, it does not absolve the student from responding to official communications sent to their University e-mail address. To forward e-mail sent to your University account, go to http://accounts.pitt.edu, log into your account, click on Edit Forwarding Addresses, and follow the instructions on the page. Be sure to log out of your account when you have finished.