**CMSE 201: Introduction to Computational Science**

**Solving problems with computers**

**Course Description**

A useful definition of *computational science* is “the use of computers to analyze and solve scientific problems.” Over the course of this semester, we will explore various aspects of computational science and will acquire a variety of practical, fundamental computational skills. In addition, we will explore application-driven modeling of various systems, with applications to the physical, life, and social sciences, and also to engineering and mathematics. While we will learn some computer programming over this semester, the goal is utilitarian – this is a course in applied computing, rather than a course intended for beginning computer science majors!

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

1. Gain insight into physical, biological, and social systems through the use of computational algorithms and tools.
2. Write programs to solve common problems in a variety of disciplines.
3. Identify salient features of a system that can be codified into a model.
4. Manipulate, analyze, and visualize datasets and use this data to evaluate models.
5. Have an understanding of basic numerical methods (e.g., numerical integration, difference equations, Monte Carlo) and be able to use them to solve problems.
6. Be able to take results from a scientific computing problem and present it both verbally and in writing.

We will work toward the goals expressed above throughout this course using a range of activities – primarily by writing software both individually and in small groups, but also through discussion, presentations, and other types of exercises.

**Topics covered**

The primary topics covered in this course include:

* Creation of models (making mathematical representations of systems).
* The basics of functional programming (i.e., variables and types, functions, simple data structures (strings, lists, dictionaries)
* Plotting and data visualization
* File and dataset manipulation
* Basic numerical techniques, possibly including statistics, linear regression, difference equations, Monte Carlo, agent-based modeling, numerical integration

Please note that **creating models to describe and understand systems** (whether they are in the physical, life, or social sciences, or in engineering) is the driving principle of this course – everything else we teach you is in service to this goal!

**Required reading materials**

This class has no required book or course pack. From time to time we will direct you toward online resources, but the main materials will be lecture notes and software.

**Other required materials**

In-class programming assignments are a critical part of the learning process in this course. To that end, you are expected to bring your laptop, power cord, and VGA adapter (to plug into the LCD projector) to class every day.

**Course activities**

**Class participation:** Active class participation (led both by the instructor and by students) is critical to the success of this course. As such, you are expected to attend class every week, bring the required materials (most importantly, your computer and power cord) and to actively participate in the in-class discussion.

**In-class programming assignments:** Class will be taught twice a week, and will be broken up into sets of mini-lectures and programming assignments that will allow you to immediately implement (and get instant feedback on) what you have just learned. In-class programming assignments will be turned in at the end of the day via DropBox.

**Programming homework:** You will have periodic programming assignments (roughly weekly) that will provide a more in-depth exploration of the materials covered in class. These will be pursued either individually or in pairs, and will be turned in by the deadline via DropBox.

**Group project:** The purpose of the group project is to provide you an extended hands-on experience with solving a scientific problem using the methods taught in this course. Over the course of the semester, you will propose a project relating to the material discussed in this course, and will act as a local expert on this topic if necessary. You will give a presentation and demonstration of your project at the end of this semester. Information on all aspects of this project appears later in the syllabus.

**Course meeting time and location**

Class will meet in LOCATION on DAYS from TIMES. The final exam session is on DAY AND DATE, and may be used for final presentations.

**Grading information**

There are a variety of course activities, with point totals as listed. More detailed descriptions of each activity can be found elsewhere in the syllabus. Note that these point totals are approximate, and may vary somewhat depending on the pace of the class. As a result, the grading scale percentages will remain constant, but the points listed may change.

Activity Points

Participation and attendance (5 points/week) 70

In-class programming assignments (5 points/week) 70

Programming homework (10 points/week) 140

Research Project proposal (w/presentation) 20

Research project status update presentation 20

Final version of research project 80

Research project final presentation 40

Total: 440 points

**Grading scale**

4.0 ≥ 90% (396 points)

3.5 ≥ 85% (374 points)

3.0 ≥ 80% (352 points)

2.5 ≥ 75% (330 points)

2.0 ≥ 70% (308 points)

1.5 ≥ 65% (286 points)

1.0 ≥ 60% (264 points)

0.0 < 60%

Note: grades will not be curved - your grade is based on individual effort, not comparative effort!

**Class attendance**

This class is heavily based on material presented and worked on in class, and it is critical that you attend and participate fully every week! Therefore,class attendance is absolutely required. An unexcused absence will result in zero points for the day, which includes the in-class programming assignment points. *Arriving late or leaving early without prior arrangement with me counts as an unexcused absence.* Note that if you have a legitimate reason to miss class (such as job, graduate school, or medical school interviews) you must arrange this ahead of time to be excused from class. Three unexcused absences will result in the reduction of your grade by one step (e.g., from 4.0 to 3.5), with additional absences reducing your grade further by one step per two absences.

**Other important information**

**Course Website and Calendar**: This course uses a GitHub page to distribute course materials, which can be found at LOCATION. Accompanying course information, including the course calendar, can be found at this website. All assignments will be handed in via DropBox. You can get an account for free, and can share individual sub-folders with Prof. O’Shea. Consult the class website for instructions.

**Classroom behavior**: Respectful and responsible behavior is expected at all times, which includes not interrupting other students, turning your cell phone off, refraining from non-course-related use of electronic devices, and not using offensive or demeaning language in our discussions. Flagrant or repeated violations of this expectation will result in ejection from the classroom.

**Email:** At times, we will send out important course information via email.  This email is sent to your MSU email address (the one that ends in “@msu.edu”).  You are responsible for all information sent out to your University email account, and for checking this account on a regular (daily) basis.

**Academic Honesty:** Intellectual integrity is the foundation of the scientific enterprise. In all instances, you must do your own work and give proper credit to all sources that you use in your papers and oral presentations – any instance of submitting another person’s work, ideas, or wording as your own counts as plagiarism. This includes failing to cite any direct quotations in your essays, research paper, class debate, or written presentation. The MSU College of Natural Science adheres to the policies of academic honesty as specified in the General Student Regulations 1.0, Protection of Scholarship and Grades, and in the all-University statement on Integrity of Scholarship and Grades, which are included in Spartan Life: Student Handbook and Resource Guide. Students who plagiarize will receive a 0.0 in the course. In addition, University policy requires that any cheating offense, regardless of the magnitude of the infraction or punishment decided upon by the professor, be reported immediately to the dean of the student's college.

It is important to note that plagiarism in the context of this course includes, but is not limited to, directly copying another student’s solutions to in-class or homework problems; copying materials from online sources, textbooks, or other reference materials *without citing those references* *in your source code or documentation*, or having somebody else do your in-class work or homework on your behalf.

**Accommodations:** If you have a university-documented learning difficulty or require other accommodations, please provide me with your VISA as soon as possible and speak with me about how I can assist you in your learning. If you do not have a VISA but have been documented with a learning difficulty or other problems for which you may still require accommodation, please contact MSU’s Resource Center for People with Disabilities (355-9642) in order to acquire current documentation.

**Instructor information**

**Contact information**

Professor:

Brian O’Shea

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Office Number and location

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**Office hours**

Professor O’Shea’s office hours are scheduled to be from TIME1 to TIME2 on DAY(S) in LOCATION. Mr/Ms. Grad Student’s office hours are scheduled to be from TIME1 to TIME2 on DAY(S) in LOCATION. Meetings outside of these times can be scheduled via email – contact either Prof. O’Shea or Mr/Ms. Grad Student to set this up.

Please note that either Prof. O’Shea or Mr./Ms. Grad Student can help you with questions pertaining to the course material, including in-class and homework assignments. If you have questions pertaining to missed classes, illness, VISA issues, or other similar things, please contact Dr. O’Shea.

**Tentative Course Calendar**

Class is on Mondays and Wednesdays, from 9:10-10:50 a.m.

Mon. 1/11: Course intro / What is a model? (Building simple models.)

Wed. 1/13: Basics of programming: program elements

Mon. 1/18: no class (Martin Luther King day)

Wed. 1/20: Making Models, II

Mon. 1/25: Programming basis, II, variables and simple programs

Wed. 1/27: Programming basics III, control structures

Mon. 2/1: P.B. IV, more control structures

Wed. 2/3: Input/output and file manipulation, I

Mon. 2/8: Input/output and file manipulation, II

Wed. 2/10: Data visualization, I

Mon. 2/15: Data visualization, II

Wed. 2/17: Working with functions, I

Mon. 2/22: Working with functions, II

Wed. 2/24: Making models, III: now with programs.

Mon. 2/29: Lists, tuples, and NumPy

Wed. 3/2: Dictionaries and sets

Mon. 3/7: no class (Spring break)

Wed. 3/9: no class (Spring break)

Mon. 3/14: Putting it all together: numerical statistics

Wed. 3/16: Numerical statistics, II

Mon. 3/21: Numerical Integration

Wed. 3/23: Numerical differentiation

Mon. 3/28: Making models, IV: predator-prey systems

Wed. 3/30: Agent-based modeling I: flock of birds

Mon. 4/4: Agent-based modeling II: digital evolution

Wed. 4/6: Monte Carlo, I: integration

Mon. 4/11: Monte Carlo, II: simple probabilistic models

Wed. 4/13: Linear regression: fitting models to data

Mon. 4/18: Small-group project day, I

Wed. 4/20: Small-group project day, II

Mon. 4/25: Class presentations, I: examples of modeling in science/egr./etc.

Wed. 4/27: last day of class. Class presentations, II

Week of 5/2: final exam (date/time/location TBD)