Syllabus: Introduction to Scientific Modeling
Spring 2018

Matthew R. Lakin

January 12, 2018

Course Information

Course title: Introduction to Scientific Modeling.
Course number: CS365.
Course credits: 3.
Class meeting days: Tuesdays and Thursdays.
Class time: 3:30–4:45pm.
Class room: Centennial Engineering Center room 1028.
Semester: Spring 2018.

Instructor

Name: Matthew Lakin.
Email: `mlakin@cs.unm.edu`
Office phone: (505) 277-3351.
Office hours: by appointment.
Office: Farris 3240.

Course description

This course is an informal introduction to the application of computational modeling as a tool for analyzing scientific data and making predictions based on that analysis. The course and course examples will use the Python programming language. As such, the early part of the course will offer a brief overview of Python programming in general, and of the libraries used for the examples in the course.

The course will cover case studies of modeling applied to a range of scientific problems from the physical, biological, and chemical sciences. There will be a particular focus on modeling the kinetics of biomolecular interactions in various situations and at various levels of abstraction, including analysis of gene expression levels in regulatory networks and predicting the behavior of engineered molecular systems.

The course is intended for advanced undergraduate students, but graduate students are welcome as well. Experience with Python is helpful but not required. No knowledge of the specific scientific concepts used as examples will be assumed, but basic knowledge of scientific and mathematical fundamentals will be helpful.

The course will consist of lectures, occasional written, modeling, and programming assignments, and examinations.

Course goals

- Students know basic principles and concepts in scientific modeling.

- Students understand the tools used to carry out scientific modeling tasks.

- Students know basic principles of the case studies covered.

Student learning outcomes

- Students can define the basic principles and concepts in scientific modeling.

- Students can select and apply appropriate tools to carry out scientific modeling tasks.

- Students can describe basic principles of the case studies covered.

Textbook and course materials

The Python programming component of the course will broadly follow the textbook:

- "A Primer on Scientific Programming with Python (5th edition)" by Hans Petter Langtagen (ISBN: 978-3-662-49886-6).

This textbook can be downloaded for free in PDF format via the UNM network, from:

- https://link.springer.com/book/10.1007%2F978-3-662-49887-3

All lecture materials will be made available via UNM Learn.

The UNM Learn email list functionality will be used for administrative announcements.

Course requirements

You are expected to attend class regularly, <u>read any assigned reading before class</u>, and participate in class discussions.

Short written and/or programming homework assignments will be given to consolidate lecture material. In the early part of the course, these tasks will be drawn from the general domains of mathematics, science, and engineering, to practice programming skills; in the later part of the course the tasks will be drawn from the case studies covered in class.

There will be two <u>in-class, closed book</u> midterm exams.

Instead of a final exam there will be an <u>individual final project</u>, which will draw on the tools and techniques covered in the course to model and analyze the behavior of biological and chemical systems.

Grading

Final grades will be based on the sum of all possible course points. The contributions of homeworks, exams, and final projects to the overall course grade will be as follows:

- Homeworks: 50%

- Exams: 30% (15% for each midterm)

- Individual final project: 20%

Grading option change requests will not be considered after the last class period.

Course schedule

The topics covered in class will be divided into three parts and will be a subset of the following, time permitting:

- Part one: Introductory Python programming

    - Python programming introduction

- basics of Python syntax
- control flow, functions
- Python modules
- object-oriented programming in Python
- Python libraries for scientific computation
- Python libraries for data visualization

- Part two: Theoretical preliminaries

  - mathematical preliminaries
  - ordinary differential equations
  - numerical integration
  - Newtonian mechanics
  - mass action chemical kinetics
  - stochastic simulations
  - stochastic and deterministic simulations of chemical reaction networks
  - the chemical master equation
  - high-level languages for biomolecular modeling (e.g., process calculi)

- Part three: Case studies in scientific modeling

  - basics of DNA biochemistry and molecular biology
  - gene regulatory networks
  - synthetic biology
  - DNA strand displacement networks
  - oscillators (e.g., Lotka-Volterra, predator-prey, repressilator)
  - partial differential equations
  - reaction-diffusion systems (e.g., Turing patterns)
  - cellular automata
  - modeling nucleic acid structures
  - nucleic acid sequence design

The schedule of activities is subject to change. Minor changes will be announced in class, major ones provided in writing.

Accommodation statement

In accordance with University Policy 2310 and the Americans with Disabilities Act (ADA), academic accommodations may be made for any student who notifies the instructor of the need for an accommodation. It is imperative that you take the initiative to bring such needs to the instructors attention, as he/she are not legally permitted to inquire. Students who may require assistance in emergency evacuations should contact the instructor as to the most appropriate procedures to follow. Contact Accessibility Resource Center at 277-3506 for additional information.

Title IX statement

In an effort to meet obligations under Title IX, UNM faculty, Teaching Assistants, and Graduate Assistants are considered "responsible employees" by the Department of Education (see pg 15 - http://www2.ed.gov/about/offices/list/ocr/docs/qa-201404-title-ix.pdf). This designation requires that any report of gender discrimination which includes sexual harassment, sexual misconduct and sexual violence made to a faculty member, TA, or GA must be reported to the Title IX Coordinator at the Office of Equal Opportunity (http://oeo.unm.edu). For more information on the campus policy regarding sexual misconduct, see: https://policy.unm.edu/university-policies/2000/2740.html

Academic integrity statement

Each student is expected to maintain the highest standards of honesty and integrity in academic and professional matters. The University reserves the right to take disciplinary action, up to and including dismissal, against any student who is found guilty of academic dishonesty or otherwise fails to meet the standards. Any student judged to have engaged in academic dishonesty in course work may receive a reduced or failing grade for the work in question and/or for the course.

Academic dishonesty includes, but is not limited to, dishonesty in quizzes, tests, or assignments; claiming credit for work not done or done by others; hindering the academic work of other students; misrepresenting academic or professional qualifications within or without the University; and nondisclosure or misrepresentation in filling out applications or other University records.