CS 365: Introduction to Scientific Modeling  
Spring 2018  
Matthew R. Lakin  
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Course Information

Lectures

Tuesdays and Thursdays, 3:30–4:45pm.  
Centennial Engineering Center room 1028.

Instructor

Matthew Lakin.  
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Office hours: by appointment.  
Office: T.B.A.

Course topics and format

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.

Assignments

There will be two in-class midterm exams. There will be a final exam covering the entire course. Several short written homework assignments may be given to consolidate lecture material. In addition, several programming assignments may be given: 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 example domains covered in class.

Course materials

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

- 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.

Grading

You are expected to attend class regularly, read any assigned reading before class, and participate in class discussion. The grade will be determined as follows:

- Homeworks: 50%
- Exams: 50% (15% for each midterm, 20% for the final)

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

The Loboweb email list functionality will be used for administrative announcements. Lecture notes and homework assignments will be circulated via email, and will also be uploaded to the UNM Learn page for the class.

Topics

The topics covered in class will be a subset of the following:

- 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

- Case studies in scientific modeling
  - 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)
  - 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

UNM statement of compliance with ADA

Qualified students with disabilities needing appropriate academic adjustments should contact the instructor as soon as possible to ensure their needs are met in a timely manner. Handouts are available in alternative accessible formats upon request.

UNM statement regarding Title IX

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