# MA579 Course Syllabus

Numerical Methods in the Biological Sciences T/TH 3:30-4:45PM, PSY B37

### **Instructor Information:**

Samuel Isaacson (<u>isaacsas@bu.edu</u>)
Professor
Department of Mathematics and Statistics
665 Commonwealth Ave., Room 442 (CDS building)

# Course Webpage:

We will use the course Blackboard site available at https://learn.bu.edu for all course material.

### Office Hours:

To be determined based on student schedules once registration is settled. For the first week of classes I will have an office hour on Wednesday 9/3 from 2-3pm in CDS 442.

# **Useful Textbook(s):**

We will primarily use class and internet-based lecture notes, but I will try to provide references where I know of them for class material. Numerical ODE solver information, our first mathematical topic, is available in:

R. LeVeque, Finite Difference Methods for Ordinary and Partial Differential Equations: Steady-State and Time-Dependent Problems, SIAM, 2007. (For numerical methods and analysis.)

- Note, this book is available to download for free through the BU library: here.

### **Description and Goals:**

This course introduces students to the use of numerical methods for studying mathematical models of biological systems. An emphasis will be placed on the development of these methods; understanding their accuracy, performance, and stability; and their application to the study of biological systems. Students will learn to program in Julia, develop mathematical models of biological systems, and understand the issues that arise in the numerical approximation of these models. Methods studied will include those for solving and parametrizing ordinary differential equations, partial differential equations, and simulating continuous-time stochastic processes. These methods will be applied to investigate mathematical models of virus dynamics, gene expression, search processes for DNA binding sites, molecular transport, and action potential propagation.

### **Prerequisites:**

MA 226 or 231 or the equivalent. Elementary knowledge of linear algebra. Prior programming experience in one of C, C++, Java, Julia, Matlab, Python, R or a related language is required. No biology background is required.

# **Programming:**

Computer assignments will use the Julia programming language.

Instructions will be available on Blackboard for setting up Julia and Visual Studio Code for editing / writing Julia code. If you'd like to get started before we use it in class please install Julia 1.11.6 from <a href="https://julialang.org/downloads/">https://julialang.org/downloads/</a>. You can start learning about the language by going through the "Introduction to Julia" tutorial at <a href="https://julialang.org/learning/">https://julialang.org/learning/</a>, and/or watching the associated Julia Youtube tutorial linked in the instructions on the course webpage. We will go through a Julia for scientific computing tutorial during the second week of class.

### **Grading:**

5% - Class participation and engagement

- Attending and participating in class.
- Asking questions in office hours.
- Keeping phones, computers, and tablets put away during lecture.

35% - Computational homework assignments.

60% - Three in class exams.

## Lecture Information:

- You are generally expected to attend class and take notes I do not normally have nice lecture notes that can be distributed. If you miss class due to illness or other reasons, please get a copy of any lecture material you missed from a fellow student.
- During lectures, cell phones and computers must be put away. Tablets are allowed only if being used for note taking.

### **Homework Information:**

- You may work together with other students on completing the homework, or use Al tools such as GPT and Claude Code to assist you in writing code. However, the final pdf report you submit must be written in your own words and demonstrate *your* understanding of the problem solutions.
- If you worked with another student or used AI tools for any homework problems, please include a short statement on how they were used at the start of your assignment.
- Computational assignment solutions should be submitted on Gradescope as one pdf file with the problems written
  up neatly, in order, with answers clearly indicated. This should include clear labeling and captioning of any figures
  or tables that are reported as part of the assignment. More detailed instructions will be provided as part of each
  assignment.
- Homework will not be accepted late except in exceptional circumstances (illness), however, the lowest homework grade will be dropped.
- Homework assignments will include analytical (i.e. pen + paper) problems that will not be collected or graded. It is expected that you will work on these as they will be covered on exams.
- Homework will generally be posted on Thursday or Friday, and due at 11:59pm one or two weeks later.
- I will post homework solutions shortly after the due date (for both computational and non-collected analytical problems).

# Exam Dates and Information:

Exams will be held on 10/2, 11/6, and 12/9.

- There will be three in-class exams, covering all lecture and homework material (both graded computational portions and non-graded analytical portions).
- The lowest exam grade will be replaced by its average with your highest exam grade.
- Students are expected to be able to attend all lectures for the course, and as such, make up exams are only given
  under exceptional circumstances (e.g. illness). Approved make up exams will generally be oral exams answering
  questions on a blackboard. If you feel you have an exceptional reason you will miss one of these exam dates
  please notify me the first week of classes.

# **Academic Conduct:**

All students are expected to know and abide by BU's code of academic conduct, see: <a href="http://www.bu.edu/academics/policies/academic-conduct-code/">http://www.bu.edu/academics/policies/academic-conduct-code/</a>

# Tentative Course Outline (\* denote possible topic)

### Week 1:

Formulation of SIR Infectious Disease Models Analytical Solution Methods Finite Difference Approximations Leading to Euler's Method Analytical Solutions to Euler's Method and Convergence

# Week 2:

Introductory Julia Labs
Implementation of Euler's Method
Application to HIV-1 Dynamics

\* Parameter Estimation

\* Forward Sensitivity Analysis

# Week 3:

Ordinary Differential Equation Models of Gene Expression and Regulation Need for Higher Order Accuracy in Models for Gene Expression and Regulation Runge-Kutta Methods Bistability and Oscillations in Feedback Regulation Using Runge-Kutta Methods

#### Week 4:

Stochasticity in Gene Expression Continuous Time Jump Process Models Analytical Solution Techniques in Simple Cases

# Week 5:

Gillespie Method Numerical Studies of Gene Expression Models, Bimodality vs. Bistability and Population Heterogeneity

### Week 6:

Jump Process Approximation Methods for Diffusion and Drift-Diffusion Processes

#### Week 7:

Diffusion in 1D and as a Model of Movement on DNA Exit Time Problems, Time to Find Binding Sites by 1D Diffusion Euler's Method for Solving the Diffusion Equation, Explicit Solution

# Week 8:

Accuracy and Stability for Euler's Method Need for Implicit Methods, Crank Nicholson Accuracy and Stability of Crank Nicholson Application of Crank-Nicholson to 1D Diffusion

### Week 9:

Molecular Motor Based Transport, Fokker-Planck Equations Exit Time Problems, Time to Travel Across Microtubules

### Week 10:

Discretization Methods for Fokker-Planck Equations, Preservation of Equilibrium Hodgkin-Huxley Cable Equation Models; Derivation, Physical Significance

# Week 11-12:

Discretization Methods for Hodgkin-Huxley Equations Hodgkin-Huxley Equation Solution Behavior for Physical Examples