PHYS 123A (Fall 2017): Computational Modeling for Physical Sciences

Instructor: Arvind Baskaran (baskaran@brandeis.edu)
Office Hours: Tuesdays 2pm - 4pm (Abelson 332) or by appointment

Grading Policy:
Homeworks (70%) and Final Exam (30%).

Required Course Work:
Homework will be assigned on LATTE at the intervals of once every one to two weeks. The homework will be announced in class and posted on LATTE with a specified due date (typically 1 week from date of assignment). No late homeworks will be accepted.
Students who miss the exams will not be granted a make-up exam unless there is documented medical or other emergencies.

Course Description:
Since the invention of computers the use of computational modeling and simulations have revolutionized the way we study physical systems. Their applications range from physics and materials science to neuroscience and ecology. These techniques are useful not only for purely theoretical endeavors but also for interpreting and guiding experimental explorations.

Theoretical descriptions of physical phenomena take the form of mathematical models. Solving these models gives us the ability to predict the consequences of changes in the physical parameters of a system. For example, one might ask through systematic simulations: “does the system behave differently at low temperature in comparison to high temperature?” This in turn allows us not only to understand experimental discoveries but also guide future experiments. However, the usefulness of such a theory is limited by one’s ability to solve the mathematical models. Thus the burden of ensuring, that a model builds in the correct physics while simultaneously ensuring that solutions of the so developed models are accessible (analytically or numerically), falls squarely on the shoulders of a computational scientist.

This course addresses the interdisciplinary needs of a computational scientists. The course aims to bridge the gap between physical sciences and applied mathematics in the context of computational modeling. Starting with the mathematical preliminaries we will discuss the techniques in developing computational models and the development of methods to solve the models.
This is done by addressing the following 3 points:
1) Ensuring the mathematical models have the correct physical features (e.g.: conservation of mass, entropy production, etc..)
2) Ensuring the correct equilibrium behavior of the models (e.g.: are there steady states, are they stable or unstable, etc.).
3) Development of computational methods to predict long term non-equilibrium behavior of the models.

The course will consist of a lecture component and a laboratory component where the mathematical methods will be implemented on a computer.
Learning Goals: Students will learn:
- the basic methods of developing mathematical models for physical systems that take the form of ordinary differential equations and partial differential equations.
- numerical and analytical techniques to understand and analyze the properties of the models including identification of fixed points and linear stability analysis of a fixed point.
- methods to numerically solve the models using finite difference methods and spectral methods to explore the non-linear evolution of the systems.

Prerequisites: Math 22a or 15a, Math 22b or 20a, Math 37a (Math 35a is recommended by not required)
Differential Equations and Linear Algebra are a requirement. A familiarity with Fourier Series/Transforms will be useful but not required. Some introduction to computer programming will also be very beneficial but the course will be self contained and teach required programming skills.

Co-requisite: EL94a Computational Modeling Lab is strongly recommended particularly for students who lack a strong background in programming. Implementation of computational methods in the form of a computer program is an integral part of the course. The programming aspects will only be covered in EL94a.

4-Credit Course: Success in this 4 credit hour course is based on the expectation that students will spend a minimum of 10 hours of study time per week in preparation for class (readings, homework, preparation for exams, etc.)

Students with Disabilities: If you are a student with a documented disability on record at Brandeis University and wish to have a reasonable accommodation made for you in this class, please contact me immediately.

Academic Integrity: You are expected to be familiar with, and to follow, the University’s policies on academic integrity. Please consult Brandeis University Rights and Responsibilities for all policies and procedures. All policies related to academic integrity apply to in-class and take home projects, assignments, exams, and quizzes. Students may only collaborate on assignments with my permission. Allegations of alleged academic dishonesty will be forwarded to the Director of Academic Integrity. Sanctions for academic dishonesty can include failing grades and/or suspension from the university.

Syllabus:

Unit 0: Examples and Motivation for Computational Modeling

Unit I: Introduction to Time Dependent Continuum Models

1) Mathematical Preliminaries, Norms, Inner Products
2) Predator Prey Dynamics, Oscillators and Ordinary Differential Equations (ODE) based models
a) ODE’s.  
b) System of differential equations and steady states  
c) Linearization, stability of steady states, phase portraits  
d) Exploring phase portraits using Matlab  

3) Introduction to Finite Difference methods 
   a) Forward Euler Method for ODE’s  

4) Landau-Ginzburg/Variational Models (Partial Differential Equation (PDE) models)  
   a) Mathematical preliminaries of variational models  
   b) Model A (Non-conserved flow on free energy surface)  
   c) Model B (Conserved flow on free energy surface)  
   d) Long time stability through energy decay  

5) Real world examples of Landau-Ginzburg Models  
   a) Modeling Phase Transitions (Allen Cahn, Cahn Hilliard Models)  
   b) Multiscale models for solidification/Pattern formation (Swift Hohenberg, Phase Field Crystal model)  
   c) Construction of Forward Euler Methods PDE models  

Unit II: Analyzing Time Dependent Models Using Fourier Series  

1) Introduction to Fourier Series  
2) Exact solution of time dependent models in Fourier space  
   a) Solution of Linear Models (Diffusion)  
   b) Understanding diffusion in a mathematical model  
      A) Stabilizing role of diffusion  
   c) Linear Stability Analysis (LSA) of Non-linear Models  
      A) Linearized Models.  
      B) Identification of fixed points.  
      A) LSA of Allen Cahn, Cahn Hilliard, Swift-Hohenberg  

Unit III: Numerical Methods for Differential Equations (As applied to models in Unit I)  

1) Preliminaries, Difference Approximations, discrete norms, order of accuracy  
2) Initial Value Problems (ODE’s)  
   a) Forward Euler, Backward Euler Methods for time dependent models  
   b) Stability of Forward and Backward Euler Methods  
   c) Runge Kutta Methods  
4) Boundary Value Problems/ Characterizing equilibriums and steady states  
   a) Solving Linear Systems of Equations  
   b) Jacobi and Gauss-Seidel Methods  
3) Finite Difference Methods for Initial Value Problems for Landau-Ginzburg models  
   a) Forward Euler Method  
   b) Backward Euler Method  
   c) Discrete Fourier transforms/ Spectral methods  
      - Preliminaries of Discrete Fourier Transforms  
      - Solving Landau-Ginzburg Models using Spectral Methods  
         - Forward Euler, Backward Euler, Crank Nicholson Time stepping methods
d) Introduction to convex splitting, un-conditional stability and unique solvability of computational methods

Unit IV: Some More Applications

1) Turing Instability in reaction diffusion equations
2) Simple models for Active Soft Matter Systems (systems of self propelled particles)
   a) Simple examples from Toner and Tu theory
3) Simple Models from Neuro Science
   a) Hodgkins Huxley / Coupled Oscillator Models for Neurons

Additional Topic: (May be covered time permitting)
Ising Model, Hydrodynamics models, Percolation Models,

Text Book:

There is no required text book for this course. Notes will be provided periodically through out the duration of the course. Some suggested reading for the different units will be assigned for from the textbooks (listed below) for those who wish to strengthen their understanding beyond the material presented in the classroom. These reading assignments will be optional but highly recommended.

Suggested Reading:

Computational Methods (Units I, II, III)

Fourier Methods (Unit II)