ME/MS 526, Simulation of Physical Processes
Fall 2024, **Tue/Thur, 1:30-3:15 pm (CDS 262)**

Instructor: Prof. James Bird
Email: jbird@bu.edu
Office Hours: **Thur. 3:15-4:15 PM (EMA 202E, 730 Comm. Ave.)**

Prerequisites: It is expected that all students have taken undergraduate courses where physical processes are modeled with partial differential equations.
Undergraduate Prerequisites: Senior or graduate standing in the engineering, physics, or the chemistry disciplines, or consent of instructor.

Course Description: Modern simulation methods are covered for describing and analyzing the behavior of realistic nonlinear systems that occur in the engineering and science disciplines. By developing and applying such methods and tools, much deeper understanding, insight, and control of novel technologies can be gained, thereby often greatly aiding technology development, and sometimes providing the leverage to turn a novel technology into a practical reality. Physical and numerical changes of scales necessary for modeling macro-, meso-, and nanoscopic phenomena will be covered. Advanced numerical methods will be addressed for attacking nonlinear partial differential equations, as well as key aspects of the finite element method. Extensive use will be made of the modern computational tool COMSOL. Same as MS 526. Students may not receive credit for both.

Course Outcomes:
Upon successful completion of this course, the aim is for students to:
1. Have a comfort and familiarity with a Multiphysics PDE solver (specifically COMSOL) to simulate a range of physical processes that are relevant to other graduate courses, industry, and research.
2. Develop a deeper understanding of how to describe diverse physical systems using ordinary and partial differential equations in scalar, vector, and tensor form.
3. Understand various sources of numerical and physical instabilities, including those resulting from propagation errors, transport errors, and nonlinearity.
4. Be able to non-dimensionalize equations and incorporate them into simulations.
5. Recognize analogous dynamics across different physical processes, especially related to canonical PDEs (eg hyperbolic, parabolic, elliptic).
6. Understand the differences and relative advantages of various numerical techniques.
7. Develop skills with various data visualization techniques.

Instructions for connecting to COMSOL on campus & remotely:
You can connect to COMSOL through on-campus computers or citrix. This link has directions on how to access citrix remotely. http://www.bu.edu/engit/knowledge-base/citrix/citrix-how-to/
You will also need to be connected to the Boston University vpn to access citrix. To connect you will need to use cisco AnyConnect. Instructions for access are here:
https://www.bu.edu/tech/services/cccs/remote/vpn/use/

Course Books & Resources:

1) COMSOL Documentation
   https://doc.comsol.com/6.2/docserver/#!/com.comsol.help.comsol/helpdesk/helpdesk.html
   - COMSOL Multiphysics Reference Manual
   - CFD Module User's Guide (For Multiphase Flow Interfaces)

   [You can get pretty far without looking at the manuals, but they will be a great resource for your final projects]
2) Application Gallery – https://www.comsol.com/models [step-by-step instructions for different example models with accompanying documents for context]
3) Olver. 2014. "Introduction to Partial Differential Equations", Springer. [This book is **available for free** online from our library https://www.bu.edu/library/]
4) Press, Teukolsky, Vetterling, Flannery (2007) "Numerical Recipes", Cambridge University Press [You do not need to purchase the book, as the material we'll discuss is freely available online http://numerical.recipes/book]

Course Blackboard Site: Used for class announcements, information, assignments, review material, additional notes, discussion forums, and schedule.

Gradescope: Used for submission of graded work and can be accessed directly or through our Blackboard site.

Course Communication: Questions about course material and assignments should be brought up in office hours, discussions, during appropriate lecture times, or posted to the Pronto discussion board (access available through Blackboard). For some reason, I often miss direct messages on Pronto, so if you would like to ask me a question in private, please send it to me by email. If an emailed question to me seems widely relevant, I may post it to the Pronto discussion board (anonymized).

Grading:
Class Participation (5%)
Homework & Group Presentation (45%)
Test (10%)
Class Project & Final Presentation (40%)

Class Participation: During the presentation of material in lectures, there will opportunities to participate through asking and answering questions or sharing insight. This engagement is encouraged and is noted in the class participation portion of grading.

Reading Assignments: Whenever possible, readings from our course material that are relevant to class topics will be noted on the Course Schedule. Students are encouraged to familiarize themselves with material to fully engage in classroom discussions.

Homework: Four or five problem sets will be posted on Gradescope around one week before their due dates. Some problem sets should be completed individually, whereas other assignments should be completed within a group. If it is not clear whether a particular homework is an individual or group assignment, please ask me.

Groups for homework and class project: Groups will be 2 to 4 people. You are welcome to pick your own groups up to a certain date, after which I will randomly form groups from the remaining folks. Your group will submit a joint assignment on Gradescope. If there are problems in groups working together, please try to work them out. If need be, talk to me and I will try to help resolve the difficulty.

Group presentation: You will be assigned to a separate group of 4 to 6 people to gather information on a topic assigned to you (eg. "What are the key differences between the finite difference method, finite volume method, and finite element method, and when might one method be better than the others?"). You will then prepare a 15-minute presentation and share it with the class during part of our regularly scheduled class time.

Test: There will be a test during the semester, as listed in the schedule. This test will take place during part of the regularly scheduled class time. It is expected that everyone will be able to take the test during its scheduled time. Arrangements or an alternative time will be made on a case-by-case basis for documented emergencies or University conflicts (**7 days prior arrangement**).

- Students requiring additional time or other accommodations must supply proper documentation from the Office of Disability Services **at least 7 days in advance** of an exam.

Class Project & Final Presentation:
Your final project is to take a concept highlighted in another class and develop a COMSOL simulation that provides insight into this concept in a style similar to those in the Application Gallery. In addition to submitting the COMSOL .mph file, you will submit a report that includes (1) context for the concept and simulation at a level appropriate for students in the targeted course, and (2) step-by-step instructions on how to set up the simulation. You are welcome to discuss your ideas with a faculty member who might teach the targeted material and you could certainly prepare your report as a "simulation lab" for students within that course to complete assuming no previous simulation experience. Finally, your group will have approximately 15 minutes to present your project to our class. Final project presentations will take place on the last two days of class. For fairness, everyone's slides will be due on the first day of presentations and the final reports due on the second day of presentations.

Policy on collaboration: Collaboration is required for group work and encouraged for non-group homework. For non-group work, students must turn in their own work in their own words. No collaboration is permitted on the test.

Generative AI Assistance Policy:
Our course follows the policies on using Generative AI in Coursework that were developed by the Faculty of Computing & Data Science.
https://www.bu.edu/cds-faculty/culture-community/gaia-policy/

Following that policy, students are expected to:

1. Use AI tools wisely and intelligently, aiming to deepen understanding of subject matter and to support learning.
2. Give credit to AI tools whenever used, even if only to generate ideas rather than usable text or illustrations.
3. When using AI tools on assignments, please (a) save the entire AI exchange and be prepared to turn it in if requested. Please also provide a description of (b) precisely which AI tools were used (e.g. ChatGPT private subscription version or DALL-E free version); (c) an explanation of how and why the AI tools were used (e.g. to generate ideas, turns of phrase, elements of text, long stretches of text, lines of argument, pieces of evidence, maps of conceptual territory, illustrations of key concepts, etc.), and (d) an account of why AI tools were used (e.g. to save time, to surmount writer's block, to stimulate thinking, to handle mounting stress, to clarify prose, to translate text, to experiment for fun, etc.).

Health and Safety: Students should not attend in-person events if feeling unwell or tested positive for COVID 19 over the last 5 days or wear facemasks. Students and instructor are expected to be aware and follow all University guidelines, recognizing that these may change throughout the semester. Please alert the instructor as soon as possible if accommodations are needed.

Diversity and Inclusion: We consider our classrooms to be a place where you will be treated with respect, and we welcome individuals of all ages, backgrounds, beliefs, ethnicities, genders, gender identities, gender expressions, national origins, religious affiliations, sexual orientations, ability – and other visible and nonvisible differences. All members of this class are expected to contribute to a respectful, welcoming and inclusive environment for every other member of the class. If something was said in class, discussion, or office hours that made you feel uncomfortable, please either let me know or tell a trusted person (e.g. academic advisor) who can relay your concerns to me anonymously. My goal is to provide everyone with the best learning experience possible.

Religious accommodations: We are aware of and in agreement with Boston University's Policy on Religious Observance, whereby absences for any religious beliefs are understood and missed assignments on such occasions will be given a chance to be made up. We require advanced notification at least a week for such occasions.

Boston University Academic Conduct Code:
Honesty is a core value of Boston University. Any violations of BU academic honesty and integrity standards will be pursued through appropriate University channels. This includes, but is not limited to cheating, plagiarism, and misrepresentation. Academic misconduct is conduct by which a student misrepresents his or her academic accomplishments or impedes other students' opportunities of being judged fairly for their academic work, which includes any help from online tutoring services during tests. Knowingly allowing others to represent your work as their own is as serious an offense as submitting another's work as your own. If you have any questions

as to what constitutes an honor code violation, please ask. ***Ignorance is not an excuse for cheating***. BU's Academic Conduct Code:
http://www.bu.edu/academics/policies/academic-conduct-code/

Auditing the course:
For graduate students who wish to audit this course rather than take it for a grade, you can fill out the appropriate audit sheet (see the MechEng front office for more information). If you choose this option, evidence of auditing the course will appear on your transcript, but you will not receive academic credit. If you chose this option, the only expectation would be that you would attend class and participate fully.

Drop and Withdrawal Dates:
Last day for graduate students to change standard courses from credit to audit status
or for anyone to DROP class (with no 'W' on your record): Oct. 8, 2024
Last day to WITHDRAW (with a 'W' on your record): Nov. 12, 2024

Incompletes:
Incompletes will be permitted only for extenuating circumstances and must be arranged Prof. Bird as soon as such a circumstance arises. This situation only pertains to assignments whose due dates have not yet passed.

ME/MS 526, Simulation of Physical Processes

The following is an approximate schedule for the course. As this is the first time that I've taught this course, the schedule is likely to be adjusted as the appropriate pacing becomes clearer.

Note: PDE 1 = "Intro to Partial Differential Equations" by Olver, Chapter 1
RM 1343 = COMSOL Reference Manual 6.2, p. 1343
NR 17 = "Numerical Recipes" by Press et al., Chapter 17
AG Lorenz = Application Gallery – Lorenz model

Date	Topic	Reading	Assignment
Sept 3	Class 1: Overview – Analytic vs numeric solutions		
Sept 5	Class 2: ODE/PDE terminology, Simulating initial value problems in COMSOL	PDE 1 RM 1343	HW #1
Sept 10	Class 3: Parameter sweeps & plotting in COMSOL	AG Lorentz	
Sept 12	Class 4: Finite difference methods, Sensitivity to numerical tolerance vs perturbation	PDE 5.1 NR 17 RM 1442	
Sept 17	Class 5: Linear homogeneous vs inhomogeneous Simulating BVPs, Heat Equation	NR 18	
Sept 19	Class 6: Species mass transfer equations Surface reaction & convective BCs	AG Spherical transport	
Sept 24	Class 7: Navier Stokes & Navier Equations Non-dimensionalizing equations & BCs		
Sept 26	Class 8: Transport PDEs. Method of characteristics	PDE 2.1-2.2	HW #2
Oct 1	Class 9: Wave equations in solid compression, water waves, & acoustics + nonlinear transport	AG Kdv PDE 2.3-2.4 PDE 8.4-8.5	
Oct 3	Class 10: Shocks, Application Builder Eigensolutions for linear equations Functions as Fourier series	PDE 3.1-3.2, AG Shock T	
Oct 8	Class 11: Bounded heat and wave equations Electromagnetic, Gravity equations	PDE 4.1-4.2 AG PaceM	
Oct 10	Class 12: Schrödinger equation Laplace, Poisson & Helmholtz Equations	PDE 4.3-4.4 AG Cone QD	HW #3 + Project Proposal
Oct 15	**NO CLASS – MONDAY SCHEDULE**		
Oct 17	Class 13: Fluid instabilities, Stability analysis, & Crank-Nicolson	AG RayBen 5.2-5.3	
Oct 22	Class 14: AMG vs GMG Methods CFL Condition	AG Karman 5.4-5.5	Presentation: Group 1
Oct 24	Class 15: Weak form vs. strong form	PDE 10.1- .2	HW #4
Oct 29	Class 16: FEM vs FVM Methods	NR 20 PDE 10.3-.4	Presentation: Group 2
Oct 31	Class 17: Boundary PDEs Surface tension, surface reactions	AG Reactor	
Nov 5	Class 18: Phase-field and level-set	AG Separate	Presentation: Group 3
Nov 7	Class 19: Nonlinear material & geometry		

Nov 12	Class 20: ALE Methods		Presentation: Group 4
Nov 14	Class 21: Green's functions & infinite boundaries	PDE 6.1-6.3	HW #5
Nov 19	Class 22: Infinite boundaries – BEM Methods	PDE 11.5, 12.3	Presentation: Group 5
Nov 21	Class 23: Test + State variables	AG PhaseChg	Test
Nov 26	Project Check-In (via zoom)		
Nov 28	**NO CLASS - THANKSGIVING**		
Dec 3	Wrapping everything up		
Dec 5	Final Project Presentations Day 1 EVERYONE's Slides due by 10:30am		Presentation slides
Dec 10	Final Project Presentations Day 2		Final Report

Initial Resources for Group Presentations:

1. AMG vs GMG Methods

https://www.comsol.com/blogs/using-the-algebraic-multigrid-amg-method-for-large-cfd-simulations
https://www.comsol.com/blogs/on-solvers-multigrid-methods

2. FEM vs FVM Methods
https://www.comsol.com/blogs/fem-vs-fvm

3. Level Set vs Phase Field Methods
https://www.comsol.com/blogs/two-methods-for-modeling-free-surfaces-in-comsol-multiphysics

4. ALE Methods
https://www.comsol.com/blogs/model-deforming-objects-with-the-arbitrary-lagrangian-eulerian-method

5. BEM Methods

https://www.comsol.com/blogs/how-to-create-electrostatics-models-with-wires-surfaces-and-solids

https://www.comsol.com/blogs/how-to-use-the-boundary-element-method-in-acoustics-modeling