Boston University, College of Engineering

Course title: **Simulation of Physical Processes**

Course # : **me-ms526**

Related info: This course is cross-listed in Mechanical Engineering and Material Science, although students from other backgrounds in engineering and the sciences are most welcome to take the course. The use of simulation, if applied effectively, is often extremely helpful in both research and technology development in all engineering and science areas. Indeed, if you are in a company that does not use simulation to some extent, then it is likely that the product and company is not so greatly sought after and that your company has little competition to worry about. That statement may sound very odd! I intend to explain it more in class, but if the issue does not come up in the first few weeks of class, please ask!

To start thinking along these lines, consider a medium sized company. Normally to remain competitive, the company will be greatly handicapped without the effective use of simulation, as the costs of running the company are generally too large without the skillful optimization and predictive power of simulation. For a large company, one also needs these features, but the company may have the luxury, time, and energy to use simulation to also look for the real intriguing technological directions ahead that might really make a huge difference in the future.

Moreover, anyone with good simulation tools and very good physical insight, can create a patent portfolio that "rocks" and changes the industry. It does not happen often, but when it does, it is exciting to see.

We will pick up with some of these thoughts during our course, but there are plenty of technical details to talk about and sort out in addition to these rough general statements!

In recent years this course has been offered in the Spring of each year, as it is now for 2022. Classes are Tu & Th, 6:30-8:15pm, in room 210 at 8 Saint Mary's Street (Photonics Building).

If you are a distance learning (DL) student, please access the class live via Zoom with coordinates (link will be posted on blackboard also):

Meeting ID 999 7281 8091 Passcode: 851170
or https://bostonu.zoom.us/j/99972818091?pwd=S0dySDJMbVJQb0RwQUFIcmxNUHNIQT09

All classes will be recorded and with permission, can be accessed if the student in class or DL student is out sick, etc., or if the DL student is granted permission to take the course this way.

Professor: Dan Cole

Contact: **email:** dccole@bu.edu (best way to contact). **Phone:** (617) 353-0432 (my cell if you really need to call me)

Office: Mechanical Engineering Department, 15 Saint Mary's Street, Rm. 133
Directions to office: Go in at 15 Saint Mary's, bear right, go down the long narrow corridor, with the glass walls on the left, through the double doors, and my office is on the left, Rm. 133. My office is very close to the ECL computer lab.

Office hours: 1:00-2:15pm on Monday and Friday. This will be done by Zoom. If you cannot make those hours, please feel free to contact me by email to arrange another time. (The link below will be posted on blackboard also.)
Meeting ID 820 5p30 4635
https://bostonu.zoom.us/j/8205304635

Catalogue description: Senior or graduate standing in the engineering, physics, or the chemistry disciplines, or consent of instructor. 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 tools Mathematica and COMSOL. Examples will be covered that include problems in micro and nanoelectronics, bioengineering, material science, photonics, and physics. Connections of these examples to sensing instrumentation and control will be made.

Discussion of the course content: The major motivation of the course is the following. Many exciting and innovative new technologies exist in a broad range of areas, such as micro and nanoelectronics, genetic engineering, robotics, photonics, bioengineering, material science, etc. A key aim of engineering is to take high-technology areas and to enable them to be turned into practical realities, *i.e.*, to make them commercially possible and manufacturable. An important means to accomplish this task is making use of modern techniques for simulating physical systems, since experimentation alone is generally an extremely expensive and time consuming approach. Consequently, if simulation methods exist that are sufficiently accurate, fast, and easy to use, then it can save considerable expense for developing technologies, improving existing ones, and making current technologies more manufacturable. All of the high-tech areas can be guided and aided, sometimes to an enormous extent, by physical simulation analysis. Sometimes developed simulation tools become sufficiently important to become an enabling component of high-technology industry. In other cases, simulation may help provide the initial decision on whether future technology directions are at all possible.

The main intent of this course is to teach modern methods of simulation of physical processes. Necessarily, the course is of a cross-disciplinary nature, since aspects of physics, chemistry, mathematics, and computational skills are required to successfully develop and apply physical simulation programs. Some of these basics will be reviewed here. Such knowledge will be incorporated when learning and using tools of modern simulation approaches, such as COMSOL (first program we will work with, spending about 2/3 of the semester on) and Mathematica, will be introduced and applied on examples of engineering and scientific interest.

Both of these programs will be made available to students in labs that can be accessed either on computers in the lab room (like ECL), or by connecting in over the internet. We will talk more about this during the first day of classes.

Examples from mechanics, to microelectronics, material science, bioengineering, manufacturing, and even product design will be attacked with simulation tools. Modelling and optimization are of course of key emphasis here, but as aided by modern, powerful simulation tools that we will push very hard on.

However, in addition, students may be surprised to learn that **real physical systems in nature** are **all** inherently nonlinear systems in nature. Only by using advanced simulation methods can we hope to gain the deepest understandings of such nonlinear systems. Likely folks have heard of a system (hurricane, tornado, rocket, machinery, or even an animal or human), as going "nonlinear"! What in the world does that mean!

In this sense, this course goes well beyond what is normally taught in undergraduate engineering and physics classes, which typically emphasize **linear systems of nature**. Why do such classes emphasize the latter? We'll explore that answer. By addressing nonlinear systems with appropriate simulation approaches, one can begin to develop deep intuitive understanding for how such systems behave. Once this understanding is gained, then engineers and scientists can develop innovative ways of using and manipulating these effects to their best advantage to help turn exciting, but initially impractical technologies, into potentially broad manufacturable technologies.

The first 2/3 of the course will be focused on learning and applying COMSOL, which contains a well-developed finite element package, to a variety of problems in the areas of stress/strain, thermodynamics, electrostatics, and fluids. These problems will be tackled by using COMSOL to solve the relevant pdes (partial differential equations) that describe such problems. When possible, comparisons will be made to analytic solutions.

In the last 1/3 of the course, we will get into nonlinear phenomena that can be described by sets of nonlinear coupled odes (ordinary differential equations). We will be using Mathematica to solve such problems. You do not need to know Mathematica at all when walking into this course, just as you do not need to know COMSOL. The book, "Nonlinear Physics with Mathematica for Scientists and Engineers," which I will next write about, does a wonderful job of both teaching Mathematica, while examining nonlinear physical and engineering related phenomena.

There will be four main sources of information that will be drawn from for information for this course. The main one is class notes. For the first two-thirds of the class, (1) class notes and (2) freely available manuals on COMSOL, that I will provide access to on-line (those are the second source of information I was referring to), will be key. In the last one-third of the class, the two sources of information will be (3) a very nice book that you could purchase, but I will provide the relevant material and chapters of in class. The full book is indeed very nice, and if you get it, you might get a used copy to save yourself some money. The book is, "Nonlinear Physics with Mathematica for Scientists and Engineers," by Richard H. Enns and George C. McGuire (a CD comes with the book, but you do not need to get it as I will supply the needed material). Lastly, (4) I will go over some material from "Numerical Recipes", by Press, Flannery, Teukolsky, and Vetterling. You certainly do not need to purchase this last book, as the material here is freely available on-line, at least for the part I want you to know: http://numerical.recipes/book .

Hence, in summary, you do not need to purchase anything, but you might consider a used copy of #3, or a new version for about $80 at say, Amazon, but only if you feel so compelled.

(1) Class notes: majority of material.
(2) Manuals of COMSOL simulation programs. There is a LOT here. I'll guide you. Don't panic! Many of you will get pretty far without ever looking at a single manual, but for your final projects, you will want these! At the moment (1/3/2022), I've placed the manuals on my google drive at:
https://drive.google.com/drive/folders/1pQcLajIlDx64q30xQAwOeDFep-jUSGbQ?usp=sharing
(I will post this on blackboard to make it easier to copy), but actually these are the manuals from last Spring and I need to update them to the latest version, and will before classes start.
(3) Material from book, "Nonlinear Physics with Mathematica for Scientists and Engineers," by Richard H. Enns and George C. McGuire.
(4) Material from, "Numerical Recipes", by Press, Flannery, Teukolsky, and Vetterling.

This course should be helpful to a wide range of other engineering and science courses and research areas. Nearly every MS and Ph.D. thesis in the engineering and science disciplines is expected to have modeling and/or theoretical support behind the effects that are being studied. More specifically, a thesis that only shows experimental data is generally not accepted. It is expected that a deeper analysis be carried out to help explain the effects observed. Simulation methods are enormously helpful here. Similarly, rarely can one publish a paper in the engineering and science journals with only experimental data being presented; generally, some deeper analysis is expected to also be presented. This course will provide the training to students along these lines, and will introduce them to the most recent tools being used.

Schedule (based on Fall / Spring semester)

Based on a total of 28 classes, with every two classes counting for 1 week of material, the following topics take up the class material. These topics do overlap with each other, as opposed to being done sequentially. The biggest split that is easiest to recognize is that the first 2/3 of the class is spent using COMSOL, and the last 1/3 is spent using Mathematica for specific nonlinear problems, and learning about nonlinear phenomena in general. Also, from the midterm on, I will be prompting you to work on your final project in parallel with class lectures and some HW, but the HW load will be lighter. Usually, it takes folks half the course to settle on what they want to pursue for a final project. I will periodically be talking about such possible final project topics and you will be presenting on such topics as well. Indeed, I will show you some past final project examples that people have done to help get your thoughts going. Don't be intimidated with the thought of "final project". Remember, you have some very powerful computational tools to tackle things you want to attack and solve! That is what makes some of this very exciting.

1. Discussion of the basic physics inherent in what we will tackle, then what it means to carry out the simulations. An initial simulation example will be given. (1 week)
2. COMSOL and the finite element method, including basic mathematics, applications, and packages. (2.5 weeks)
3. These techniques will then be applied to a variety of problems, including examples from microelectronics, nanoelectronics, bioengineering, materials science, physics, and photonics. This material will be mixed in with #2 above. (4.0 weeks).
4. Essential aspects of partial differential equations for describing physical systems, with emphasis on nonlinear equations, optimization techniques, and numerical methods for solving these problems. (2.5 weeks)
5. Use of Mathematica for solving nonlinear ODEs and understanding more about nonlinear phenomena. (3 weeks)
6. Presentation of class projects (1 week)

Homework assignments will be given throughout the course. The **grading** will be:

(1) Homework (35%)
(2) Midterm (25%)
(3) Final "quiz" (10%)
(4) Class project (30%)

For each of these you will receive a numerical grade for the four topics above. The final grade will be computed using the weights above. This grade will then be converted into a "letter" course grade in the following way: 80=>83.33 would be a B-, 83.34=>86.66 would be a B, and 86.67=>89.99 would be a B+, and likewise for the other ranges of 70=>79.99, 90=>99.99, etc.

In the first 2/3 of the course, in the Spring of 2022, we will be using COMSOL to solve four homework (HW) assignments. You will be placed on a group of peers from your class to work on these HWs. In the Spring of 2022, these four problems will consist of :

1. A steady state fluid dynamics rotational problem, with some physical symmetry boundary conditions imposed. Navier-Stokes equations will be assumed to hold! Knowing how to do this will be helping for final projects such as "lab on a chip" (biomedical diagnostics), energy gains in wind mill designs, aeronautics, etc.
2. Thermal conduction in various solid structures under steady state conditions. In this assignment, we will find both analytic solutions and numerical solutions and compare, for 1D, 2D, and 3D scenarios.
3. Thermal conduction for transient situation, where a chemical reaction occurs, as in cooking, baking, etc. We will compare to a physical model, as well as to experiment.
4. Electrostatic simulations of steady state situations for capacitors, including 2D and 3D scenarios. Here we will compare numerical and analytic results.

In the second 1/3 of the course, we will be using Mathematica on nonlinear problems and learning about nonlinear phenomena. Here I will assign the 5th HW assignment and use Mathematica to model a situation that might occur in manufacturing, where one models the probability distribution of good and bad parts coming off the line due to a variety of complex factors. A Monte Carlo modelling method will be introduced, plus an optimization technique, and two lectures will be spent on these topics plus on how the design of experiment approach (DOE) can fit in with optimizing such a situation to increase the yield (percent of "good" parts produced) in the manufacturing line. This will be the first time in me-ms526 that I have covered this topic, but is seems appropriate. Relating it to nonlinear behavior under certain conditions will be even more interesting!

In terms of dates, HWs will be due about every two weeks, until the 5th assignment is completed, partway into the last 1/3 of the course. Specific dates for each homework will be announced. Due to the size of the class, groups of probably four people will be assigned to tackle each homework. Each group will prepare ONE homework to pass in for each of the five assignments; hence, good coordination and teamwork will be important. The last 1/3 of the class will be devoted to working on the final project, which each group will present in class during the last days of our course. There will be a midterm, which will be based on lecture material. No computer/calculator will be used for this midterm. Questions will be based on material presented during class discussions and material written on the board. The midterm is intended to compliment the more computer oriented work you do for homework, to show that you understand the ideas that the simulations are based on. I will present examples of what I mean as we get closer to the midterm. However, here is one example: in COMSOL, and later in Mathematica, you can solve various **nonlinear** wave equations. Analytically, with pencil and paper, we can solve the **linear** wave equation. I'll likely show the latter derivation on the board, both the physical origin of the equation for some phenomena, and how to analytically solve the equation. I'll also explain why it would be most difficult to solve the nonlinear case without simulation methods to help us. Thus, a good question for the midterm might be for you to physically "derive the linear wave equation", using only pencil and paper, and then explain physically how nonlinear aspects can enter in, and why it would be difficult to analytically solve the resulting nonlinear equation.

I am thinking of having the midterm on either Class #13 (Tu 3/1/2022) or Class #14 (Th 3/3/2022), as there are a total of 28 classes, including the last two classes, where presentations will be taking place on final projects. We can discuss and decide later.

Each student takes their own midterm exam and final quiz, of course. All HWs, however, are submitted by the group, and all get the same grade. If there are problems in groups working together, please try to work them out (I will be offering you to pick your own groups up to a certain date, then I randomly fill in the remaining names); but of course, if need be, talk to me and I will try to help resolve the difficulty. In a big group, unfortunately, it is sure to happen.

Finally, as for final project, pick something that you find really interesting! That will enormously help motivate you! Here are the constraints: I'll give more detail when the class starts, but, basically, you can pick just about anything! Most people use COMSOL, a few folks use Mathematica, but you can use Ansys, SolidWorks with Physical Simulation, CATIA, Abaqus, etc. I don't care. Whatever you pick, use it well. Explain how you used the program to tackle your investigation and how you conducted your simulation experiments. Do they make sense in providing the information you hope to illustrate?

Lastly, it is, unfortunate, but somewhat easy to fool people with simulation, as there is just so much data that can be produced! Does it make sense? Explain. Pick your topic such that it is possible to have a check on your simulation results, either by a simple experiment, a published result by others that can be readily cited. Here is an example – Myth Busters experimentally tested the effect of a car drafting on a truck in front it, at different speeds, in terms of gas mileage. This can be done in simulation and via experiment! I expect to discuss this sort of thing a fair bit.

Your final project, as a group, only needs to be your presentation and slides. No report is required other than your slides and personal presentation. Grades are usually quite good, as people really like to get into these projects. It is really fun to see!

Dan