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 it, since simulation studies are usually quite helpful in both research and technology development in all engineering and science areas. In recent years this course has been offered in the Spring of each year, as it is now for 2021. Classes are Tu & Th, 6:30-8:15pm, in room 206 at 8 Saint Mary's Street (Photonics Building). To access the class via Zoom, please use:
Meeting ID 948 5490 3535 Passcode: 661760
or https://bostonu.zoom.us/j/94854903535?pwd=YW9jQ04rSjkxcGpQeHlmakNUTmQ0Zz09

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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 posted on blackboard.)
Meeting ID 933 9547 9986 Passcode: 186884
or https://bostonu.zoom.us/j/93395479986?pwd=V0xWWFhERTJCeFBGMDJoV1NGN3FRdz09

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 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 class.

Examples from mechanics, to microelectronics, material science, and bioengineering will be attacked with simulation tools. Students will learn that real physical systems in nature, that have true relevancy in most technologies, are inherently nonlinear in nature. Only by using advanced simulation methods can we hope to gain deep understandings of such nonlinear systems. 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. 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. As mentioned earlier, 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 two main textbooks used in this course, <u>but only the first one needs to be obtained</u>. Relevant material from the second can be obtained on-line, which I will go over. The two books are: (1) "Nonlinear Physics with Mathematica for Scientists and Engineers," by Richard H. Enns and George C. McGuire (<u>a CD comes with the book, but you do not need to get</u>

it as I will supply the needed material), and (2) “Numerical Recipes”, by Press, Flannery, Teukolsky, and Vetterling. Again, book #2 you will not need to purchase. Also, feel free to get a used copy of book #1, such as through addall.com, or other such sources. Again, you do not need the CD.

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)

Items 2-4 will not be done in sequence, but will overlap, taking up about 9 weeks combined.

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. 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 terms of dates, homeworks will be due about every two weeks, until roughly 2/3 into the course. Specific dates for each homework will be announced. Due to the size of the class, groups of three people will be assigned to tackle each homework, so, one report per group. 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 class #13 (total of 26 classes), which falls on Thursday, 3/11/21.