

## BOSTON UNIVERSITY COLLEGE OF ENGINEERING

**Course title:** Simulation of Physical Processes

**Course #:** ME/MS526 (cross-listed in Mechanical Engineering and Material Science).

Instructor: Prof. Dan Cole.

**Catalogue description:** This course covers modern simulation methods 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.

**Prerequisite:** Senior or graduate standing in the engineering, physics, or chemistry disciplines, or, consent of instructor.

### 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 exists that is 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 just mentioned can be guided and aided, sometimes to an enormous extent, by developing and applying 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. Next, tools of modern simulation approaches, such as Mathematica and COMSOL, the latter of which provides an advanced finite element package, will be introduced and applied on examples of engineering and scientific interest. Examples from microelectronics, to 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 attacking 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 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. COMSOL is a very powerful program if used properly, which is much of what we will go over. Often, when possible, comparisons will be made to analytic solutions.

In the last 1/3 of the course, we 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 ...,” which I will now talk 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, but only the first one needs to be obtained. Relevant material from the second can be obtained on-line. The two books are: (1) “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), and (2) “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)**

1. Initial simulation example from nonlinear dynamics of controlling atomic systems, then a deeper look to show what is behind all of this work. (0.5 weeks)
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. (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. (3 weeks)
5. Use of Mathematica for solving these equations combined with the use of Scientific Workplace for enabling manipulation, analysis, and presentation of material. (2.5 weeks)
6. Class projects (1.5 weeks)

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.

### **Contact:**

You can reach me at:

#### **Professor Dan Cole**

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My office is fairly close to the ME Computer lab, ECL. If unfamiliar, go into 15 Saint Mary’s (directly opposite from the Saint Mary’s entrance to Photonics), bear right, go down the long narrow corridor, past double doors, past ECL on the left, and my office, #135, is on the right.

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