Syllabus:
CPS 5310: Mathematical and Computer Modeling
Spring 2014

Instructor:
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Office hours: TR 2:00-2:50pm, others by appointment

Class time and location:
TR 6:00-7:20pm, UGLC 334

Course website: http://svmoore.pbworks.com/

Course description: Computer simulation of selected practical problems from physics, engineering, geology, biology or chemistry. Students learn to create mathematical models formulate modeling assumptions, select appropriate numerical methods, implement them in the form of a computer program, and visualize the numerical results. Emphasis is given to verification and validation procedures.

Prerequisites: Calculus and linear algebra, CPS 5401 with grade of B or better; or permission of the instructor

Textbook: *Mathematical Modeling and Simulation: Introduction for Scientists and Engineers*, Kai Velten, Wiley-VCH, 2009, ISBN: 9783527407588.
Book software website: https://sites.google.com/site/booksoftwaremms/

We will also use parts of the following online textbooks:
- Victor Eijkhout, Introduction to High-performance Scientific Computing, http://tacc-web.austin.utexas.edu/veijkhout/public_html/istc/istc.html
- Cleve Moler, Numerical Computing with MATLAB, http://www.mathworks.com/moler/chapters.html , 2004

Learning outcomes:
After successfully completing this course, students should be able to
- DESCRIBE the major approaches to mathematical modeling
- DEFINE an appropriate mathematical model for a physical problem
- DESIGN and IMPLEMENT a solution strategy for a mathematical model
- VALIDATE the results of a mathematical model
- APPLY regression models to analyze datasets
- FORMULATE and SOLVE mechanistic models of physical systems using ODEs
- FORMULATE and SOLVE mechanistic models of physical systems using PDEs
- APPLY mathematical software to solve large-scale models on high performance computer systems

Course topics:
The following is a list of topics to be discussed. The exact schedule may vary depending on previous background of class participants. Although the instructor will do some lecturing, we will try to use a "flipped classroom" format to some extent that will require reading and preparation by class participants prior to class and involve group work during class.

- Principles of mathematical modeling (textbook Ch. 1)
    - steps of modeling and simulation
    - classification of mathematical models
    - using the computer algebra software Maxima
- Phenomenological models (textbook Ch. 2)
    - descriptive statistics
    - random processes and probability
    - inferential statistics
    - linear regression
    - nonlinear regression
    - using calc and R
- Mechanistic models I: ODEs (textbook Ch. 3)
    - setting up ODE models
    - first-order ODEs
    - autonomous, implicit, and explicit ODEs
    - Initial Value Problem
    - Boundary Value Problems
    - systems of ODEs
    - solution of ODEs
- Mechanistic models II: PDEs (textbook Ch. 4)
    - theory of PDEs
    - numerical solution of PDEs
        - finite difference method
        - finite element method
    - examples
        - flow in porous mediApa
        - computational fluid dynamics (CFD)
        - structural mechanics
- High performance mathematical software
    - software for ODEs
    - software for PDEs
- Applications (tentative)
    - molecular dynamics
    - quantum chemistry
    - climate modeling
    - computational astrophysics

Assignment, exams, and grading:
There will be approximately six homework assignments. There will be one "midterm" exam, to be given approximately 2/3 of the way through the course, and a final project. The grading breakdown will be approximately as follows:

Homework	30%
Midterm exam	30%
Class preparation and participation	10%
Final project	30%

Final project:
The final project will consist of:
1. development and solution of a mathematical simulation model for a physical problem not discussed in class nor assigned for homework
2. a report describing the background for the model, model definition, simulation method, results, and validation
3. a presentation during the final exam period describing and demonstrating your model

The specific problem can be of your choosing but you must have your topic pre-approved by the instructor. You may work individually on the final project or in teams of up to three people. In the case of group work, you must do clearly document the contributions of each team member and carry out the amount and difficulty of work proportional to the size of your team.

Make-up assignments and exam:
If you are unable to attend the midterm exam or to turn in a homework assignment on time due to a legitimate reason, such as a health problem or accident or pressing family matter, you will be allowed to make up the relevant exam or assignment.

Accommodations for Students with Disabilities

If you have a disability and need classroom accommodations, please contact The Center for Accommodations and Support Services (CASS) at 747-5148, or by email to cass@utep.edu, or visit their office located in UTEP Union East, Room 106. For additional information, please visit the CASS website at www.sa.utep.edu/cass.

Academic Honesty Policy

Make sure you understand the UTEP academic honesty policy. Students are encouraged to share ideas, but you must do your own homework and you must write your own code for the projects (you may copy code that is on the course website). If homework or program code is suspected of being duplicated or copied, you will receive an incomplete for the assignment, and your case will be referred to the Dean of Students for adjudication. If the instructor has reason to believe that you have cheated on a quiz or exam, your case will be referred to the Dean of Students for adjudication.