

## CPS 5310 Syllabus, Computational Science, UTEP

Course #:	CPS 5310
Course title:	Mathematical and Computer Modeling
Credit hours:	3
Term:	Spring 2019
Time & location:	1:30-2:50pm TR, Bell Hall 130 (Lab)
Prerequisites:	Calculus III (MATH 2313), Matrix Algebra (MATH 3323), and Introduction to Computational Science (CPS 5401) with grade of B or better; or permission of the instructors.
Course fee:	None
Instructors:	Natasha Sharma and Ming-Ying Leung
Office location:	Sharma: Bell Hall Room 318 Leung : Bell Hall Room 225
Contact information:	Sharma: Office phone: 915-747-6858 Email: <a href="mailto:nssharma@utep.edu">nssharma@utep.edu</a> <a href="http://www.math.utep.edu/Faculty/nsharma/public_html/teaching.html">http://www.math.utep.edu/Faculty/nsharma/public_html/teaching.html</a> Leung: Email: <a href="mailto:mleung@utep.edu">mleung@utep.edu</a> Office phone: 915-747-6836 <a href="http://www.math.utep.edu/Faculty/mleung">http://www.math.utep.edu/Faculty/mleung</a>
Office hours:	Sharma: 12:00-1:00 pm TR or by appointment. Leung: Posted weekly at <a href="http://www.math.utep.edu/Faculty/mleung/officehours">www.math.utep.edu/Faculty/mleung/officehours</a>
Teaching assistant:	Ms. Sumi Dey
TA office location:	CCSB 2.0108A
TA email:	<a href="mailto:sdey2@miners.utep.edu">sdey2@miners.utep.edu</a>
TA office hours:	Wednesdays 1 - 3 p.m. (to be confirmed)
Online textbook:	Mathematical Modeling and Simulation: Introduction for Scientists and Engineers, Kai Velten, Wiley-VCH, 2009, ISBN: 9783527407588 Additionally, sections of the following online books will also be used: <ul style="list-style-type: none"> <li>• Victor Eijkhout, <i>Introduction to High-performance Scientific Computing</i></li> <li>• Cleve Moler, <i>Numerical Computing with Matlab</i>, 2004</li> <li>• Sheldon Ross, <i>Introduction to Probability Models</i>, 10<sup>th</sup> Edition, 2010</li> </ul>

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### 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.

### Grading

Your grade for the course will be based on the following:

- 50% homework (including labs)
- 40% midterms and final project
- 10% class preparation and participation

### Attendance Policy

**Lecture and lab attendance is required and noted at the beginning of class; more than a total of TWO unexcused absences will result in an instructor-initiated drop or final grade reduction. Your academic/research advisor will be consulted before final action is decided and taken.**

### 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](mailto: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](http://www.sa.utep.edu/cass).

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## 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.

## Course Format and Participation

The lecture portion of the class will consist of short lectures interspersed with hands-on interactive activities. Lab assignments will reinforce the lecture material. The lecture and lab exercises will make use of CS Department Linux lab machines, the UTEP Research Cloud, and the Stampede Supercomputer at Texas Advanced Computing Center. Students should be able to login to these resources remotely from a home or office computer. All students should bring a laptop computer to class with which to login to the remote resources. (Please let the instructors know if you do not have a laptop you can bring to class).

## Course Topics

The following is a list of topics to be discussed. The exact schedule may vary depending on previous background of the class participants.

1. Principles of mathematical modeling [textbook Chapter 1]
  - steps of modeling and simulation
  - classification of mathematical models
  - using the computer algebra software Maxima
2. Phenomenological models [textbook Chapter 2]
  - descriptive statistics
  - random processes and probability
  - inferential statistics
  - linear regression
  - nonlinear regression
  - using calc and R
3. Mechanistic models I: ODEs [textbook Chapter 3]
  - setting up ODE models
  - first-order ODEs

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- autonomous, implicit, and explicit ODEs
  - Initial Value Problem
  - Boundary Value Problems
  - systems of ODEs
  - numerical solution of ODEs
  - Parameter Estimation for ODEs
4. Mechanistic models I: ODEs [textbook Chapter 4]
- theory of PDEs including Euler and Lagrange equations
  - numerical solution of PDEs (finite difference and finite element methods)
  - examples (flow in porous media, computational fluid dynamics, structural mechanics)
5. High-Performance Mathematical Software
- software for ODEs
  - software from PDEs (C++ Library deal.II and Fortran Library PDE2D)

### Term project

The term project will consist of:

1. development and solution of a mathematical 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 describing and demonstrating your model,
4. model definition, simulation method, results, and validation

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

### Learning Outcomes

After successfully completing this course, students should be able to

1. DESCRIBE the major approaches to mathematical modeling
2. DEFINE an appropriate mathematical model for a physical problem
3. DESIGN and IMPLEMENT a solution strategy for a mathematical model
4. VALIDATE the results of a mathematical model
5. APPLY regression models to analyze datasets
6. FORMULATE and SOLVE mechanistic models of physical systems using ODEs
7. FORMULATE and SOLVE mechanistic models of physical systems using PDEs
8. DESIGN and IMPLEMENT solutions to models in a scientific programming language
9. APPLY mathematical software to solve large-scale models on high-performance computer systems