

## **MA 4990/6990–Simulation Modeling Spring 2013**

### **Course Description**

The goals of this course are to: (1) formulate a mathematical model describing a physical phenomenon; (2) to discretize the model; (3) design and analysis of numerical algorithms for solving equations resulting from discretization; (4) implementation of numerical algorithms; (5) performance of numerical experiments; (6) scientific visualization of the data and computational simulation in an immersive and interactive virtual reality (i.e., CAVE) environment; (7) managing large datasets.

### **Course Meetings**

TR, 11am-12:15pm, Allen Hall, Room 20 (Section 1)

### **Instructor**

Dr. Suzanne Shontz  
438 Allen Hall  
Dept. of Mathematics and Statistics  
Office Phone: (662) 325-7151  
E-mail: sshontz@math.msstate.edu

**Office Hours:** Tuesdays and Thursdays from 9:30-10:30am or send e-mail to schedule an appointment in advance. (Note that I have a second office which is A204 in the HPC<sup>2</sup> Building; at times I will be in this office and will need sufficient notice to come to campus to meet with you.)

**Note that my scheduled office hours will be updated once the class shifts to the HPC<sup>2</sup> Building. At that time, I will move my office hours to my office in the HPC<sup>2</sup> Building.**

### **Teaching Assistant**

None

### **Recommended Texts**

1. Mathematical Models in the Applied Sciences [highly recommended]

Author: A.C. Fowler

Publisher: Cambridge Press

ISBN: 0-521-46703-9

Year: 1997

2. Introduction to Parallel Computing (Second Edition)

Author: Ananth Grama, Anshul Gupta, George Karypis, Vipin Kumar

Publisher: Addison-Wesley

ISBN: 0-201-64865-2

Year: 2003

3. OpenGL Programming Guide: The Official Guide to Learning OpenGL, Versions 3.0 and 3.1 (7th Edition) [highly recommended]

Author: Dave Shreiner

Publisher: Addison-Wesley

ISBN: 0-321-55262-8

Year: 2009

### **Prerequisites**

MA 1713 (Calculus I); MA 1723 (Calculus II); MA 3113 (Introduction to Linear Algebra); One of CSE 1213, CSE 1233, CSE 1273, or CSE 1284 (for example) Introduction to Programming (in any language).

### **Course Requirements**

*Lecture attendance is required*, although attendance will not be recorded. The course requirements for MA 4990/6990 include class participation, three homework assignments (one each in modeling, simulation, and visualization), two midterm exams, and a final project to be done with a partner. The project will involve an informal midterm report, a final report, and a poster presentation. Graduate student homework and projects will be expected to be done more in-depth than undergraduate student work. Specifics as to the expectations for graduate students will be detailed on each assignment, project, or exam. The homework assignments will require a combination of mathematical modeling (formulated analytically, i.e., by hand), problem solving, algorithmic design, computer programming (using C++ or OpenGL), and scientific visualization (not all on a single assignment). *Neither prior knowledge of C++ nor OpenGL is a prerequisite for the course.*

Homework assignments will be due about ten days after they are assigned. Due dates for homework assignments will be announced in class. **There will be a late penalty of 10% for homework handed in up to 24 hours late. No homework assignments will be accepted more than 24 hours late.**

**There will be two midterm exams; the dates for the midterm exams are given on the course calendar.** Please reserve these dates on your calendar. The midterm exams will be closed-book. A make-up midterm will be given to any student who is absent from the exam for a compelling reason and gets permission from the instructor.

There will be a **final project in lieu of a final exam. The final project involves an informal midterm report, a final report, and a poster presentation. The date for submission of the final report and presentation of the poster is given on the course calendar.** A make-up final presentation will be given to any student who is absent from the poster presentation for a compelling reason and gets permission from the instructor.

The exams will cover topics drawn from the lectures and homework, and from the underlying mathematics, algorithms, and visualizations.

## **Grading**

Class participation will count for 5% of the final grade. The homework assignments will count for 25% of the final grade. The two midterm exams will each count for 20% of the final grade, and the final project will count for 30%.

## **Honors Credit**

Students may earn honors credit for the course by completing a final project with an extra component (to be agreed upon by the student and the instructor in advance) and filing a petition requesting approval of the honors designation for the course.

## **Class Schedule**

The course calendar shows a week-by-week syllabus. The dates and order of topics are subject to change by the instructor. Any significant changes will be announced in class.

## **Course Website and E-mail**

There will be a course website within MyCourses. E-mail announcements will be sent via MyCourses. **Students are responsible for checking MyCourses daily for course e-mail messages.** (Alternatively, one may choose to forward their MyCourses e-mail messages to another e-mail account which can more easily be checked.)

## **Computing Facilities**

Students will have accounts in the High Performance Computing Collaboratory (HPC<sup>2</sup> Building) for use with the computational simulation and scientific visualization components of the class. The accounts will be for writing C++ and OpenGL codes and for developing scientific visualizations. More details on these accounts will be provided soon. Earlier in the semester, the class will tour the computational facilities in the HPC<sup>2</sup> Building. The HPC<sup>2</sup> Building is in Research Park; students may drive to Research Park and park near the building (if they display a MSU parking permit). Alternatively, they may take the campus bus to the building. **Later in the semester, especially when studying scientific visualization, we will sometimes meet at the HPC<sup>2</sup> Building for lecture.**

## **Books on Reserve**

I will consider placing relevant mathematical modeling, computational simulation, and scientific visualization textbooks on reserve in the library. Note that I plan to order the course textbooks through the Department of Mathematics and Statistics yearly book allotment.

## **Academic Integrity Policy**

Mississippi State University has an approved Honor Code that applies to all students:

### **The Honor Code states:**

“As a Mississippi State University student I will conduct myself with honor and integrity at all times. I will not lie, cheat, or steal, nor will I accept the actions of those who do.” Upon accepting admission to Mississippi State University, a student immediately assumes a commitment to uphold the Honor Code, to accept responsibility for learning, and to follow the philosophy and rules of the Honor Code. Students will be required to state their commitment on examinations, research papers, and other academic work. Ignorance of the rules does not exclude

any member of the MSU community from the requirements or the processes of the Honor Code. For additional information, please visit: <http://students.msstate.edu/honorcode>.

Students are allowed to collaborate on the homework assignments with at most one other student of the class. The collaboration should involve no more than the formulation of ideas as a pair. Each student is expected to write up the homework assignment by himself or herself. Students must not hand in homework that represents somebody else's ideas entirely. Students should do the C++ or OpenGL coding on assignments by themselves--no program code should be shared. No collaboration of any kind is allowed on the midterm exams.

Students are permitted to consult outside published material for the homework, although the homework will be fully based on lecture notes, course handouts, and the textbooks. If a student consults a source other than the lecture notes and textbook, he or she must cite the source--failure to cite the source will be considered cheating.

Students will collaborate on the final project with a partner. No student will work by himself or herself. (If there are an odd number of students, one group will have three students in it.)

The penalty for cheating will be an F for the course, following a hearing with the instructor as spelled out in the university's academic honor code policy. In extreme circumstances the instructor will in addition bring the case before the university's MSU Honor Code Council.

*Suzanne M. Shontz, Mississippi State University, [sshontz@math.msstate.edu](mailto:sshontz@math.msstate.edu)*

**MA 4990/6990 – Simulation Modeling  
Week-by-Week Syllabus**

<b>Week</b>	<b>Lecture Topics</b>	<b>Notes</b>
<b>1</b>	<b>Jan. 8 and 10:</b> Introduction to Mathematical Modeling; Discrete Models	Chapter 1, Fowler. (Dr. Shontz is away on January 10. Dr. Oppenheimer will lecture that day.)
<b>2</b>	<b>Jan. 15 and 17:</b> Nondimensionalization; Asymptotics	Chapters 2 and 3, Fowler.
<b>3</b>	<b>Jan. 22 and 24:</b> ODE Models – The Belousov-Zhabotinskii reaction; Enzyme kinetics	Chapters 10 and 9, Fowler. Homework #1 handed out on January 22.
<b>4</b>	<b>Jan. 29 and 31:</b> PDE Models – Navier-Stokes equations for fluid flow problems; Solid mechanics models	Chapters 6 and 7, Fowler. Homework #1 due on January 31
<b>5</b>	<b>Feb. 5 and 7:</b> Numerical ODE algorithms: initial value problems, boundary value problems	Handout
<b>6</b>	<b>Feb. 12 and 14:</b> Numerical PDE algorithms: finite difference and finite element methods	Handout
<b>7</b>	<b>Feb. 19 and 21:</b> Geometric modeling and mesh generation	Handout
<b>8</b>	<b>Feb. 26 and 28:</b> Compression of large datasets/Midterm Exam #1	Handout/Midterm Exam #1 on February 28.
<b>9</b>	<b>Mar. 5 and 7:</b> Parallel computing – domain decomposition, scalability, analysis, MPI, etc.	Chapter 3.2, 5, and 6, Grama/Homework #2 out on March 5
<b>BREAK</b>	<b>Mar. 12 and 14 – Spring Break</b>	No class this week.
<b>10</b>	<b>Mar. 19 and 21:</b> Model/View: objects, cameras, projections; Transformation of objects and animation.	Chapter 2 and 3, Shreiner/Homework #2 due on March 21
<b>11</b>	<b>Mar. 26 and 28:</b> Lighting, materials, normals, colors, texture	Chapter 4 and 5, Shreiner
<b>12</b>	<b>Apr. 2 and 4:</b> Interaction with objects	Chapter 13, Shreiner/ Homework #3 out on April 2
<b>13</b>	<b>Apr. 9:</b> Open GL in the CAVE environment	Handout/Homework #3 due on April 11
<b>14</b>	<b>Apr. 16 and 18:</b> Visualization Toolkit (VTK)	Handout/Midterm Exam #2 on April 18
<b>15</b>	<b>Apr. 23:</b> Last Day of Class	Time to work on projects during class.
<b>FINAL</b>	<b>Thursday, May 2 – 12-3pm – Final Project Poster Session in the HPC<sup>2</sup> Building</b>	Final project poster presentation and report due