

***Engineering Science and Mechanics and
Materials Science and Engineering 5984
Computer Simulation of Mechanical Behavior of Materials
(ADP TITLE: COMP SIM MATL)***

**Location: Pamplin Hall Room 1008
Time: 2:30-3:45 pm M,W
ESM 5984 Index# 96273**

I. Catalog Description:

5984 COMPUTER SIMULATION OF MECHANICAL BEHAVIOR OF MATERIALS

Classical and advanced models predict mechanical behavior of materials; numerical models incorporate state of the art simulation techniques; simulation results span various length scales from atomistic to the continuum which use embedded atom and finite element methods; models explain how macroscopic properties are controlled by phenomena at the atomistic and microstructural levels; interpretation of models results use interactive Java Web-based and immersive virtual reality technology.

(3H, 3C). II.

ESM/MSE 5984

COMP SIM MATL

II. Learning Objectives:

Upon successful completion of this course, the student will be able to:

- understand the fundamental concepts in continuum mechanics: conservation of mass, momentum and energy,
- understand how macroscopic properties are controlled by phenomena at the atomistic and microstructural levels,
- study and analyze model predictions using advanced visualization techniques,
- compose a final project in a well organized and well designed visual format using multimedia or web software.

III. Justification:

Computer simulations have become increasingly useful for many scientific disciplines especially materials engineering . The advent of supercomputers allowed materials researchers to simulate more realistic problems in materials engineering, especially those problems that do not have exact closed form solutions. Since computing is becoming cheaper, more powerful, and easier to use, it is expected that today's materials engineering student will encounter the use of supercomputing simulations on the job. Much of the materials research in the last twenty years, that has used computer simulations, has not found its' way into the undergraduate or entry level graduate classes.

To focus on the model development and mechanics of materials research, and avoid the emphasis of computer science, this course made the use of interactive visual Java Web-based interfaces that minimized the time students spent in preparation of computer simulations. Rather students focus on parametric design, facilitated by the interactive interfaces and visual interpretation of results using Web-based visual data analysis tools. In special cases where properties are the result of complex three-dimensional structures, the CAVE is used so that students can experience these structures in total immersion.

No credit is given for developing or programming visual interfaces although it is expected that students demonstrate proficiency in programming as a prerequisite for the class project.

IV. Prerequisites & Corequisites:

Prerequisites: First year graduate student familiar with at least one programming language.

V. Text and Special Teaching Aids:

1. Class Notes on Web, and interactive Java Web-based interface to computer simulations.
<http://www.jwave.vt.edu/crcd>

VI. Syllabus:

Percent of Course

- | | |
|---|------|
| 1. Introduction to continuum mechanics: stress, strain, anisotropy (six lectures) | 20 % |
| 2. Introduction to elasticity solutions: i.e. thick-walled cylinder (three lectures) | 10 % |
| 3. Concepts in fracture mechanics: mode I, II, III, stress intensity (three lectures) | 10 % |
| 4. Wave propagation in unbounded media: isotropy vs. anisotropy (three lectures) | 10 % |
| 5. Laminated plates: singularities without cracks (three lectures) | 10 % |
| 6. Cracks at bimaterial interfaces: isotropic and anisotropic (six lectures) | 20 % |
| 8. Class project: specific problem assigned to groups | 30 % |