ME/CME/CE/ASE 8373 (MSU) AND CHEME 7700 (LSU): INTEGRATED COMPUTATIONAL MATERIALS ENGINEERING FOR METALS

Class Hours: MWF 11:00-11:50 pm Location: 100 Swalm Bldg (MSU)

Office Hours: T&Th 1:30 - 3:00 pm Location: 210 Chemical Engineering Bld. (LSU)

Instructor: Dr. Mark Horstemeyer
Nitin Sukhija, nitin@cavs.msstate.edu
Shane Brauer sbrauer@cavs.msstate.edu

Office: 206 Carpenter
Phone: 662-325-5449
Email: mfhorst@me.msstate.edu

Dr. W. A. Shelton (LSU)
Tommy Trieu: : ttrieu1@tigers.lsu.edu
Office: 210 Chemical Engineering Bld.
Phone: 225-578-3069
Email: wshelton@lsu.edu

WHY STUDY INTEGRATED COMPUTATIONAL MATERIALS ENGINEERING FOR METALS?

(1) The next-generation structures will all be based on the paradigm of simulation-based design concepts. A student will need to know the various computational tools to be competitive in the work force.

(2) By integrating the various length scale tools, a student will understand the connectivities of structure-property relationships, theory-experiment relationships, and process-performance relationships. This fundamental knowledge base will position the student for advantages in higher fidelity computations and designs.

(3) Because this technical elective will not be *boring*. It is fun and inspirational to see computational results give insight into phenomena from materials processing and performance environments.

COURSE OBJECTIVE

The primary objective of this course is to learn the process of analyzing and understanding computational tools at different length scales and how they interact with each other in terms of bridging. Although engineering products and systems can fail their design requirements allowing for new tools for efficient and effective evaluation is crucial. As such, we will cover plasticity, damage/fracture, and fatigue in the context of designing metallic structures from the view of multiple length scales. We will also examine experimental techniques for model exploration, model calibration, and model validation as well as failure prevention in the context of a diverse set of actual case studies. The case studies are used to provide a real world link for the material failure mechanisms and analysis tools you will learn in this class. It is also designed for distance learning.

COURSE PREREQUISITES

It will be critical to have undergraduate courses on the behavior of materials so that you understand the basics such as stress and strain and materials science so that you know the basic structure of materials.

TEXTBOOK AND REFERENCES

A book was written for this specific course in order to raise the awareness of ICME. Also, there exists a website in which the support information and exercises will be come from.

Book: M.F. Horstemeyer, *Integrated Computational Materials Engineering for Metals: Using Multiscale Modeling to Invigorate Engineering Design with Science*, Wiley, 2011.

Website:
https://icme.hpc.msstate.edu

MY TEACHING PHILOSOPHY

I am a firm believer that a strong course should be interesting (inspiring), practical, technically strong, challenging, and prepare you for the next steps in your learning. It is VERY important to me that you all have a positive experience from this class and you learn a lot. I will do my best to present the information is a succinct manner which is more time effective and intriguing than reading the material from a textbook or the WEB.

COURSE OPERATION (WHAT WILL YOU AND I DO?)

In teaching this course, I will try to discuss the context and usages of the multiple length scale analyses in order to provide a larger picture of the details in which the simulations will be derived. I expect that a student would get familiar with the ICME CyberInfrastructure (CI), read the book for context and clarifications, and examine the in-class lecture notes carefully. The ICME CI contributions will count for 10% of the grade, which includes additions and updates to the tutorials, results of computations or experiments, and final summaries of journal articles with associated simulation animations. Five contributions are a minimum requirement for earning the class participation grade of 10%.

The homeworks/exercises are designed to provide the foundation for the integration aspects of ICME meaning that each homework will help bridge two different length scales of simulations, and this will be the basis for the project. Homework 1 will focus on the bridge between electronics and atomistic simulations; Homework 2 will focus on the bridge between the atomistic and dislocation dynamics bridge; Homework 3 will focus on the bridge between dislocation dynamics and crystal plasticity; and Homework 4 will focus on the bridge between crystal plasticity and macroscale. Each homework problem will be worth 15% of your total grade, so all of the homework problems comprise 60% of the total grade.

The research proposal will include a write-up that defines a technical problem and all of the associated length scale simulations and bridges along with an outline of the potential paper and will be 10% of your grade. Although the homeworks and projects are based upon teams, the research proposal will be based upon an individual's work. A presentation of your work will be given publically in powerpoint.

A critical review of two articles regarding ICME will be 5% of your grade. A critical review summarizes what the authors are purporting and then you present arguments what makes it a good ICME paper or a bad one.

The final will be 15% of your grade and will be an in-class test that will comprise questions (true-false, fill-in the blank, and some essay). The questions will come from the whole course.

Research Proposal	10%
ICME CI Contributions	10%
Homeworks/Exercises	60%
Critical Review of ICME papers	5%
Final	15%

COURSE TEAMS

The homeworks will be completed in teams. Each team will consist of four-five students students.

Honor Code

Mississippi State University has an approved Honor Code that applies to all students. The code is as follows:

"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.