ISC 5229: Multiscale Modeling of Materials

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Office hours	Tuesday 10:00 am – 12:00 noon Other times by appointment
Textbook	See recommended references and reading list
Class	Tuesday, Thursday 2:00 – 3:15 pm DSL 468

Catalogue description

ISC 5229: Multiscale Modeling of Materials (3). Mathematical and algorithmic basis for atomic scale, mesoscale and continuum scale modeling approaches in materials science, emphasizing the atomic-to-continuum connection, statistical approaches and homogenization problems in continuum modeling of heterogeneous materials. Concrete examples will be used to explain the basic ideas, and the students will pursue projects in which they apply the concepts discussed in the lectures.

Prerequisites

Basic knowledge of atomic structure of materials, concepts of continuum mechanics, and graduate level knowledge in engineering mathematics or mathematical physics.

Course Objectives

At the end of the course, the students will be able to

1. identify the correct modeling technique (atomic, continuum, hybrid atomic-continuum, or homogenization) for a given materials science problem,
2. set up and implement atomic scale models of materials structure and properties,
3. carry out continuum thermomechanics models and obtain results for materials properties,
4. construct simple multiscale models involving both atomic and continuum scale models,
5. construct models for the effective properties of heterogeneous materials, and
6. identify the computational algorithms to be used to solve the above models.

List of Topics

The topics covered under this course include:

1. length and time scale aspects of materials science problems,

2. atomic and continuum scale problems of materials structure and properties,
3. hierarchical continuum scales in heterogeneous materials,
4. continuum field equations and constitutive laws: thermomechanics as an example,
5. statistical mechanics view and molecular level models,
6. connection between atomic and continuum views, derivation of continuum scale laws from molecular materials models,
7. homogenization methods in heterogeneous and random media,
8. contemporary multiscale paradigms: concurrent and hierarchical coupling of materials models at various scales, and
9. computational algorithms through term projects.

Grading Policy

The student grade for the course will be determined by homework, a midterm exam, final exam and a term project. These parts of the total grade are weighted as follows:

Homework:	25%
Midterm Exam:	25%
Term Project:	25%
Final Exam:	25%

Term Project

Following the introductory part of the course (by second week), a set of potential project subjects will be discussed in class and each student or small group of students will have the opportunity to select a project area. The students will conduct independent reading in this area for three weeks, at the end of which each student or group of students will select a simple problem of multiscale materials modeling based on consultation with the instructor. The project work involves literature assessment, selection of a simple material model for mathematical modeling and computational implementation, a written short report not exceeding 10 pages, and a final presentation at the last class meeting.

Announcements

The instructor will periodically make announcements about homework assignment and due dates, homework solution, midterm and final exams, and term projects.

ACADEMIC HONOR POLICY:

The Florida State University Academic Honor Policy outlines the University's expectations for the integrity of students' academic work, the procedures for resolving alleged violations of those expectations, and the rights and responsibilities of students and faculty members throughout the process. Students are responsible for reading the Academic Honor Policy and for living up to their pledge to ". . . be honest and truthful and . . . [to] strive for personal and institutional integrity at Florida State University." (Florida State University Academic Honor Policy, found at http://dof.fsu.edu/honorpolicy.htm.)

ADA

Students with disabilities needing academic accommodation should:
(1) register with and provide documentation to the Student Disability Resource Center; and
(2) bring a letter to the instructor indicating the need for accommodation and what type. This should be done during the first week of class.

This syllabus and other class materials are available in alternative format upon request.

For more information about services available to FSU students with disabilities, contact the:

Student Disability Resource Center
874 Traditions Way
108 Student Services Building
Florida State University
Tallahassee, FL 32306-4167
(850) 644-9566 (voice)
(850) 644-8504 (TDD)
sdrc@admin.fsu.edu
http://www.disabilitycenter.fsu.edu/

Syllabus (detailed list of topics to be covered)

1. Length and time scale aspects of materials science problems—How length and time scale issues arise in materials problems; connection of these issues with material models (atomic versus continuum); which kind of model for which material problem.

2. Atomic and continuum scale problems of materials structure and properties—Formalism of atomic scale and continuum scale problems for materials structure and properties.

3. Hierarchical continuum scales in heterogeneous materials—Microstructure hierarchy in materials and continuum-to-continuum model coupling; importance in materials response (mechanical and non-mechanical).

4. Continuum field equations and constitutive laws—Derivation of balance laws of continuum mechanics; thermodynamics and constitutive theory; thermomechanics of crystalline materials as an example.

5. Statistical mechanics view and molecular level models—Atomic/molecular view of materials response and conservation laws; statistical mechanics concepts; phase space concepts; ergodicity; statistical ensembles.

6. Connection between atomic and continuum views—Derivation of equilibrium and non-equilibrium continuum conservation laws from statistical mechanics; correspondence between atomic and continuum scale pictures of materials; mechanics and thermomechanics of crystalline materials.

7. Homogenization methods in heterogeneous and random media—Examples of heterogeneous media and homogenization (averaging) techniques for mechanical and transport properties.

8. Contemporary multiscale paradigms: concurrent and hierarchical coupling of materials models at various scales—Theoretical and computational formalism of the quasi-continuum method, coarse-grained molecular dynamics, and bridging scale techniques.

9. Computational algorithms through term projects—Concept summary of numerical tools required in solving multiscale materials problems: FEM, MD, MC, Linear and Non-linear solvers, and Optimization techniques. This section aims to establish the connection between this course and other computational science courses.

Recommended Reading List

1. J.H. Weiner, Statistical Mechanics of Elasticity, Dover Publications (2002)
2. W.K. Liu, E.G. Karpov and H.S. Park, Nano Mechanics and Materials: Theory, Multiscale Methods and Applications, Wiley (2006)
3. Rob Phillips, Crystals, Defects and Microstructures Modeling Across Scales, Cambridge University Press (2001)

4. S. Nemat-Nasser and Muneo Hori, Micromechanics: Overall Properties of Heterogeneous Materials, Elsevier (1999)
5. Instructor's handouts, citing a package of book chapters and review articles