MatSE 404ELA: Modeling Elasticity

Spring 2017

Schedule

TR 2:00–5:00pm in L440 Digital Computer Laboratory

- Lecture: 2:00–3:30pm
- Lab: 3:30–5:00pm

Meets Jan. 17–Mar. 9 (first half of semester)

Course content

- Course website: courses.engr.illinois.edu/mse404ela; PDF syllabus
- Assignment upload: my.matse.illinois.edu/courses/upload, select MSE 404 ELA
- Online in-class quizzes: PrairieLearn

Scope

- Computational materials modeling tools for predicting elastic behavior of materials
  - Crystalline materials: density-functional theory (QuantumEspresso)
  - Composite materials: finite element simulation (OOF2)
- Physical principles underlying software
- Ranges of modeling applicability and limitations
- Multiscale modeling via parameter passing

Objectives

Students will be able to

1. apply modeling tools to predict elastic behavior of new materials;
2. determine proper parameters for a simulation;
3. determine if a simulation result is reliable based on the underlying physical principles in the simulation;
4. systematically analyze data to extract meaningful materials quantities;
5. interconnect materials modeling tools to cover appropriate length scales efficiently;
6. use a command line with shell scripting to automate computational tasks.
Prerequisites: Senior standing in MatSE

- Introductory Solid Mechanics
  - MSE 206, or equivalent (TAM 251)
- Mechanical behavior of Materials
  - MSE 406, or equivalent
- Structure and phases of materials
  - MSE 201, or equivalent
- Electronic Properties of Materials/Condensed Matter Physics
  - MSE 304, PHYS 460/560, or equivalent.
- Helpful: prior experience with command line interface, and/or a programming language

Instructor

Dallas R. Trinkle (dtrinkle@illinois.edu; 308 MSEB in the west stairwell).

- Associate Professor (joined Univ. Illinois in 2006)
- Computational materials science
  - Crystalline defects (dislocations, point defects, interfaces) from density functional theory
  - Development of new algorithms, computational tools
  - Solid solution softening / strengthening, pipe diffusion, general theory of diffusion
- Office hours: by appointment only

Teaching approach: Hands-on project-based learning

An “active learning” approach where we focus on the course objectives: applying modeling tools to predict elastic behavior of new materials, determine if a simulation is reliable, and use a systematic approach to computation. You will:

- Practice using computational tools to predict elastic constants;
- Determine appropriate simulation parameters using systematic techniques;
- Automate your calculations and analysis using scripts;
- Integrate computational methods to bridge length scales;
- Communicate your results and understanding in written form.

We will apply this to predicting the elastic moduli of a metal matrix composite including the effect of size, shape, and elastic anisotropy of the reinforcement in the spirit of integrated computational materials engineering (ICME).
Logistics

• Classes will consist of
  – in-class lecture/discussion about theory and practical aspects
  – hands-on lab including walkthroughs and time for the projects.

• The classroom is reserved Tues/Thurs 2:00–4:50pm to be available to you to work on this course, even if there is not a lecture scheduled on that day.

• There may be times when “laboratory” time is used to makeup missed lectures.

• Lecture time will also include in-class quizzes to assess your understanding of the theoretical and practical material.
  – In-class quizzes are open notes, and will be available in-lecture on PrairieLearn.

Projects

For each topic, you will turn in projects along with a final project that integrates your work to study a metal-matrix composite.

• Projects
  – include a detailed brief describing the specific goals and deliverables;
  – end with a short report detailing their findings;
  – build up the pieces for your final project.

• Final project
  – integrates and builds on your work from the entire semester;
  – culminates with a detailed (5–8 page) report;
  – includes an Abstract, Introduction, Methods, Results and Discussion, Conclusions, Bibliography;
  – graded on
    1. design of computational materials research project (20%),
    2. appropriate and competent use of computational tools (50%), and
    3. clarity of the report (30%)

Project uploading

• All assignments are deposited electronically, and late submissions will not be accepted.
• In case of illness, personal crisis (e.g., car accident, required court appearance, death of a close relative), or required attendance at an official UIUC activity (e.g., varsity athletics, band concert), you must contact Prof. Trinkle well before the due date.
• Assignment upload: my.matse.illinois.edu/courses/upload, select MSE 404 ELA
Grading

Breakdown:

- **10%** Quizzes
- **20%** Project 1 (bash): **due Jan. 26**
- **20%** Project 2 (Quantum Espresso): **due Feb. 16**
- **20%** Project 3 (OOF2): **due Mar. 9**
- **30%** Final project (integrated study of MMC): **due Mar. 16**

Letter grades: A (>90), B (>80), C (>70), D (>60).

Academic Integrity, Harassment, and Discrimination

You are bound by the University Honor Code in this course. Any violation of the Honor Code will result in disciplinary action.

Students are responsible for producing their own quiz answers and project reports. Collaborative interaction in small groups is encouraged, but each student must perform all calculations themselves, and write their own reports. **Plagiarism will not be tolerated, and verified incidents will result in all parties receiving a zero and formal academic sanctions.** Students are responsible for familiarizing themselves with the definition of and penalties for plagiarism in Section I-401 of the UIUC Student Code. Note that plagiarism includes “copying another student’s paper or working with another person when both submit similar papers without authorization to satisfy an individual assignment.”

**Harassment or discrimination of any kind will not be tolerated.** Please report any concerns immediately to your professor.

Changes to syllabus

May occur as deemed necessary by the professor; they will be announced and the updated syllabus posted on the course website.

Calendar

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<thead>
<tr>
<th>Tuesday</th>
<th>Thursday</th>
<th>notes</th>
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<tbody>
<tr>
<td>Jan 17</td>
<td>Jan 19</td>
<td>Introduction / bash</td>
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<tr>
<td>Jan 24</td>
<td>Jan 26</td>
<td>Quantum Espresso theory + practice</td>
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<tr>
<td>Jan 31</td>
<td>Feb 02</td>
<td>Quantum Espresso walkthrough + project</td>
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<td>Feb 07</td>
<td>Feb 09</td>
<td><em>no class</em>; project</td>
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<tr>
<td>Tuesday</td>
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<td>notes</td>
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<tr>
<td>Feb 14</td>
<td>Feb 16</td>
<td>OOF2 theory + practice</td>
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<tr>
<td>Feb 21</td>
<td>Feb 23</td>
<td>OOF2 walkthrough + project</td>
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<td>Feb 28</td>
<td>Mar 02</td>
<td>no class; project</td>
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<tr>
<td>Mar 07</td>
<td>Mar 09</td>
<td>Final project</td>
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**Online reading**

You may want to use the following references throughout the course:

- Quantum Espresso manual
- OOF2 manual

**Accessing library resources**

The Univ. Illinois library has access to a huge variety of electronic resources; this plus additional online resources will be our references. Many can be accessed from the library’s website, or via the campus VPN. Alternatively, you can take advantage of the library proxy. This is done by appending proxy2.library.illinois.edu to the web address; when reloaded, you will be asked for Univ. Illinois authentication, and then will be able to access the resource as if you were on campus. In general, this authentication is required only once per session. So, the website


would become

http://journals.aps.org.proxy2.library.illinois.edu/prl/abstract/10.1103/PhysRevLett.113.025504

Alternatively, install the Proxy Bookmarklet which makes it extremely easy to use the proxy. I highly recommend this method.