

MatSE 404ELA: Modeling Elasticity

Spring 2021

Schedule

TR 9:00–10:50am on Zoom + CampusWire + Gather.town

Meets Jan. 26–Mar. 18 (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).

- 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.
- We will use EWS remote login: see EWS Lab Remote Access
- **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 Feb. 4**
- **20%** Project 2 (Quantum Espresso): **due Feb. 18**
- **20%** Project 3 (OOF2): **due Mar. 11**
- **30%** Final project (*integrated study of MMC*): **due Mar. 18**

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

Formal and Informal Accommodations

I am committed to assisting students requiring special accommodations for circumstances that are registered with the DRES Student Services Department. These formal accommodations should be discussed with me as early as possible in the semester or as soon after DRES approval as possible.

If you are not formally registered with DRES and have anxiety, depression, learning disabilities, or other issues that affect your ability to fully participate and learn in this class, you are encouraged to check-in with me so we can determine together the kind of support you need to thrive in this class. Please set up a meeting with me via email.

Inclusion and Diversity

I value all students regardless of their background, race, religion (creed), ethnicity, gender, gender expression, age, country of origin, disability status, marital status, sexual orientation, or military status, etc., and am committed to providing a climate of excellence and inclusiveness within all

aspects of the course. If there are aspects of your culture or identity that you would like to share with me as they relate to your success in this class, I am happy to meet to discuss. Likewise, if you have any concerns in this area of facing any special issues or challenges, you are encouraged to discuss the matter with me (set up a meeting via email) with an assurance of full confidentiality (only exception being mandatory reporting of academic integrity / code violation and sexual harassment). **Harassment or discrimination of any kind will not be tolerated.**

Anti-Racism and Inclusivity Statement

The intent is to raise student and instructor awareness of the ongoing threat of bias and racism and of the need to take personal responsibility in creating an inclusive learning environment.

The Grainger College of Engineering is committed to the creation of an anti-racist, inclusive community that welcomes diversity along a number of dimensions, including, but not limited to, race, ethnicity and national origins, gender and gender identity, sexuality, disability status, class, age, or religious beliefs. The College recognizes that we are learning together in the midst of the Black Lives Matter movement, that Black, Hispanic, and Indigenous voices and contributions have largely either been excluded from, or not recognized in, science and engineering, and that both overt racism and micro-aggressions threaten the well-being of our students and our university community.

Learning Environment

The effectiveness of this course is dependent upon each of us to create a safe and encouraging learning environment that allows for the open exchange of ideas while also ensuring equitable opportunities and respect for all of us. Everyone is expected to help establish and maintain an environment where students, staff, and faculty can contribute without fear of personal ridicule, or intolerant or offensive language. If you witness or experience racism, discrimination, micro-aggressions, or other offensive behavior, you are encouraged to bring this to the attention of the course director if you feel comfortable. You can also report these behaviors to the Bias Assessment and Response Team (BART) bart.illinois.edu. Based on your report, BART members will follow up and reach out to students to make sure they have the support they need to be healthy and safe. If the reported behavior also violates university policy, staff in the Office for Student Conflict Resolution may respond as well and will take appropriate action.

Religious Observances

Illinois law requires the University to reasonably accommodate its students' religious beliefs, observances, and practices in regard to admissions, class attendance, and the scheduling of examinations and work requirements. You should examine this syllabus at the beginning of the semester for potential conflicts between course deadlines and any of your religious observances. If a conflict exists, you should notify your instructor of the conflict and follow the procedure at ODOS to request appropriate accommodations. This should be done in the first two weeks of classes.

Sexual Misconduct Reporting Obligation

The University of Illinois is committed to combating sexual misconduct. Faculty and staff members are required to report any instances of sexual misconduct to the University's Title IX Office. In turn, an individual with the Title IX Office will provide information about rights and options, including accommodations, support services, the campus disciplinary process, and law enforcement options.

A list of the designated University employees who, as counselors, confidential advisors, and medical professionals, do not have this reporting responsibility and can maintain confidentiality, can be found here: wecare.illinois.edu/confidentiality.

Other information about resources and reporting is available here: wecare.illinois.edu.

Family Educational Rights and Privacy Act (FERPA)

Any student who has suppressed their directory information pursuant to Family Educational Rights and Privacy Act (FERPA) should self-identify to the instructor to ensure protection of the privacy of their attendance in this course. See FERPA info for more information on FERPA.

Academic Integrity

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 work. Collaborative interaction is encouraged, but each student must do their own individual prelecture work, and contribute their own work to the group. **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."

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

Tuesday	Thursday	notes
Jan 26	Jan 28	Introduction + bash ; Project 1 / PDF
Feb 02	Feb 04	Quantum Espresso theory + practice ; Quantum Espresso walkthrough/PDF
Feb 09	Feb 11	Project 2 / PDF
Feb 16	Feb 18	OOF2 theory + practice ; OOF2 walkthrough/PDF
Feb 23	Feb 25	Project 3 / PDF
Mar 02	Mar 04	project

Tuesday	Thursday	notes
Mar 09	Mar 11	Final project / PDF
Mar 16	Mar 18	project

Quiz dates in **bold**: Feb. 4, Feb. 11, Feb. 25

Online reading

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

- **Review of anisotropic linear elasticity and composite moduli**
- *The Linux command line: a complete introduction*, William E. Shotts, Jr. (San Francisco : No Starch Press, 2012.): e-book
- *Linux Shell Scripting With Bash*, K. O. Burtch (Sams Publishing, 2004): e-book
- C. Newham *Learning the bash Shell: Unix Shell Programming* (O'Reilly Media, Inc., 2009): e-book
- M. F. Horstemeyer *Integrated Computational Materials Engineering (ICME) for Metals: Using Multiscale Modeling to Invigorate Engineering Design with Science* (Wiley, 2012): e-book
- 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

`http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.113.025504`

would become

`http://journals.aps.org.proxy2.library.illinois.edu/prl/abstract/10.1103/Phy`

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