MENG 24300
Molecular Modeling
Spring 2023

Instructor: Prof. A.L. Ferguson
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CRN: MENG 24300 (100 units)

Lecture: KPTC 101 ◆ 12:30–13:50 CST ◆ Tue, Thu

Discussion: ERC 381 ◆ 17:00-18:00 CST ◆ Thu – Instructor office hours
Hinds 184 ◆ 12:30–13:20 CST ◆ Wed – TA office hours

Dates: 03/20/2023 – 06/03/2023

Course Summary

This course will introduce students to the methods of quantum and classical molecular modeling and simulation. The course will be delivered primarily through project-based learning using popular quantum mechanical electronic structure (e.g., Quantum Espresso) and classical mechanical molecular dynamics (e.g., Gromacs, LAMMPS) simulation packages. Students will also develop proficiency in the command line interface and shell scripting. The course will prioritize the physical principles underlying the methods to confer an understanding of their applicability and limitations, and hands-on immersive praxis to give students the confidence and expertise to independently use these tools.

Prerequisites

- [**REQUIRED**] MENG 21300 - Engineering Quantum Mechanics
- [**REQUIRED**] MENG 21400 - Molecular Engineering Thermodynamics
- [**REQUIRED**] MATH 18300 - Mathematical Methods in the Physical Sciences I
  or MATH 19620 - Linear Algebra
  or MATH 21100 - Basic Numerical Analysis
  or STAT 24300 - Numerical Linear Algebra
  or MATH 20250 - Abstract Linear Algebra
- [**RECOMMENDED**] Familiarity with Linux and shell scripting useful but not required

Required Text

None.

Secondary Texts

M. Garrels *Introduction to Linux (3rd ed.)* (Fultus Corporation, 2010)
K.O. Burtch *Linux Shell Scripting With Bash* (Sams Publishing, 2004)
C. Newham *Learning the bash Shell: Unix Shell Programming* (O'Reilly Media, Inc., 2009)

A. Szabo *Modern Quantum Chemistry: Introduction to advanced electronic structure theory* (Dover, 1996): https://catalog.lib.uchicago.edu/vufind/Record/2596803

D. Frenkel and B. Smit *Understanding Molecular Simulation: From algorithms to applications* (Academic Press, 2002): https://catalog.lib.uchicago.edu/vufind/Record/11155428

Quantum-Espresso Manual: www.quantum-espresso.org/users-manual
LAMMPS Manual: http://lammps.sandia.gov/doc/Manual.html
Gromacs Maunual: https://manual.gromacs.org/documentation/

Attendance

Lecture: Lectures will be split between (i) traditional instruction covering the mathematical underpinnings of the numerical tools, (ii) immersive project-based learning. **Attendance to the lectures is expected.**

Discussion: The discussion section serves as TA office hours and an opportunity for additional time to work on hands-on exercises and projects. This time may occasionally be used to provide make-up lectures.

Assessment

As a hands-on class, competence and proficiency will be assessed through (i) projects associated with each course module, (ii) short online quizzes, and (iii) a student-defined term project. **There will be no written midterm or final examinations.**

Quizzes: Short, online multiple-choice quizzes will be issued to gauge understanding and mastery of the mathematical and algorithmic principles underlying the numerical techniques. Quizzes will be available online for a specified time period, and solutions posted after the quiz closes. **Accordingly, no extensions can be granted.**

Topic Projects: Projects associated with each topic are a primary means of instruction and assessment for the course. Students will be provided with a project brief comprising a list of learning objectives, problem statement, solution approach, and set of deliverables. **Late submissions will not be accepted, but students with legitimate requests for extensions should contact Prof. Ferguson well in advance of the due date.**

Term Project: Students will design and execute a short individual research project on a student-defined topic in computational materials science and engineering using one of the molecular modeling packages covered in class. Students may select from a list of potential project topics or choose their own.

Topic – Prof. Ferguson will be available to discuss and advise topic selection. Submissions should take the form of a one-sentence topic title and short abstract that (i) summarizes the topic area and its importance, (ii) defines specific objectives and how they will be achieved using computational tools. Early topic identification is encouraged.

Report – Term project reports should be approximately 5 pages in length (excl. figures and bibliography; 12-pt font, 1-inch margins, single-spaced). Papers should be structured as a short lab report containing the following sections: Abstract, Introduction, Methods, Results and Discussion, Conclusions, Bibliography. Term projects will be graded on (i) design of computational materials research project (20%), (ii) appropriate and competent use of computational tools (50%), and (iii) clarity of the report (30%). **Late submissions will not be accepted, but students with legitimate requests for extensions should contact Prof. Ferguson well in advance of the due date.**

Exams: None.

Grading

Breakdown:

Quizzes	5%
Project 1 (bash)	20%
Project 2 (Quantum-Espresso)	20%
Project 3A (LAMMPS)	20%
Project 3B (Gromacs)	20%
Term Project	15%

Letter Grades: Letter grades will be based on final aggregate student scores, with numerical cutoffs specified by the instructor. However, students with aggregate scores >95% are guaranteed *at least* an A, >85% *at least* a B, and >75% *at least* a C (i.e. cutoffs for these letter grades will not be higher than these values).

Canvas

Course announcements, materials, grades, quizzes, and projects will be posted via Canvas (https://canvas.uchicago.edu). Online quizzes and projects will be submitted via this portal. It is students' responsibility to check Canvas for announcements and updates. Canvas is best viewed using Chrome or Firefox web browsers; Safari is known to have issues.

Slack

We will be using Slack as a virtual and public forum for questions discussion. The system allows for fast responses from the instructor, TA, and classmates, and permits students to see previous questions and answers. Rather than emailing questions to the teaching staff or using Canvas chat, please post your questions within the appropriate channel on Slack. If you have not already been automatically enrolled, please sign up via https://meng24300-spring2023.slack.com

Plagiarism

Students are responsible for producing their own quiz answers, code to solve projects, and project reports. Collaborative small group interactions are 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 awareness of the definition and penalties for plagiarism in the Student Manual (https://studentmanual.uchicago.edu/academic-policies/academic-honesty-plagiarism/). Further details on what does and does not constitute plagiarism is available here: https://internationalaffairs.uchicago.edu/page/honest-work-and-academic-integrity-plagiarism

Disability Statement

University of Chicago is committed to ensuring equitable access to our academic programs and services. Students with disabilities who have been approved for the use of academic accommodations by Student Disability Services (https://disabilities.uchicago.edu) and need a reasonable accommodation to participate fully in this course should follow the procedures established by SDS. Timely notifications are required in order to ensure that your accommodations can be implemented. Please set up a time to meet with the instructor to

discuss your access needs in this course after you have completed the SDS procedures for requesting accommodations.

Equity, Diversity, and Inclusion Statement

The Pritzker School of Molecular Engineering advances the mission of translating advances in basic physics, chemistry, biology, and computation into new tools to address important societal problems and to create a research and teaching environment that enhances and transmits these capabilities to future generations. The school affirms a commitment to equity, diversity, respect, and inclusion, and aims for broad representation, accountability, and participation among our faculty, other academic appointees, research and administrative staff, and students across age, gender, race, nationality, ethnicity, socioeconomic status, sexual orientation, ability and disability, religion, belief, and backgrounds. For resources for the PME community, as well as a how-to guide on reporting bias, please visit https://pme.uchicago.edu/equity-diversity-inclusion.

Laptop Computer

As a hands-on computational course, a laptop computer will be very useful in permitting students to follow along and run scripts and code live during course lectures. If you do not have access to a laptop computer and would like one for the duration of the course, please contact the course instructor to discuss arrangements for a possible loan.

Course Coverage

0. Introduction: CMSE / ICME

Computation as the "third pillar" of science; introduction to molecular modeling and simulation; multi-scale and multi-physics computation; drivers in academia, industry, and public policy; computational materials science and engineering (CMSE) and integrated computational materials engineering (ICME); resources and software tools

I. Scripting in scientific computing: bash shell

Command line interface (CLI) and graphical user interface (GUI); common bash commands; shell scripting utilities (expr, ssh/scp, sftp, vim, wget); installing software from source; bash scripting through worked examples; awk

Project 1: *weather watcher – wget, if, case, awk, loops*

II. Electronic structure: Quantum-Espresso

Theory*: review of quantum mechanics – Schrodinger, Hartree, Hartree-Fock, DFT; particle in a box; hydrogen atom and electronic orbitals; basis set expansion; many-electron problem; Slater determinants; exchange and correlation; Hohenberg-Kohn Theorems; Kohn-Sham equations; exchange-correlation functionals; pseudopotentials; Bloch Theorem; plane wave basis set; reciprocal space; Brillouin Zone; k-points sampling; band structure plots; successes and failures of DFT; post-DFT methods*

Praxis (Quantum Espresso)*: functionality; documentation and tutorials; installation; parallel performance; high-level overview of running QE from the command line; input/output files; convergence criteria; visualization*

Walkthrough*: H_2 molecule – ab initio prediction of energy and bond length*

Project 2*: Al xtal – convergence, energy, lattice parameter, modulus, and band structure*

III. Molecular dynamics: LAMMPS & Gromacs

Theory*: molecular dynamics as a "computational microscope"; applications in academia and industry; history and milestones; Laplace's Demon / clockwork universe; quantum effects; initial configuration and velocity; interaction potentials / force fields; Verlet algorithm; MD in various ensembles – thermostats and barostats; periodic boundary conditions; Ewald summation; specialized MD variants; successes and failures of MD; MD software packages*

(A) Praxis (LAMMPS)*: availability; installation; documentation; performance; anatomy of a LAMMPS simulation; visualization in OVITO*

Walkthrough*: Al xtal – cohesive energy, lattice parameter, and crack propagation*

Project 3A*: Al xtal – Young's modulus and Peierls stress*

(B) Praxis (Gromacs)*: availability; installation; documentation; performance; anatomy of a Gromacs simulation; visualization in VMD*

Walkthrough*: Magainin antimicrobial peptide – solvation; equilibration; structure and dynamics*

Project 3B*: Trp Zip β-Hairpin – non-equilibrium unfolding and Jarzynski equality*

Tentative Schedule

Class	Date	Day	Module	Topic	Due
1	Mar 21	T	0 / I	Intro to molecular modeling + shell scripting – theory	
2	Mar 23	R	I	shell scripting – praxis + project	
	Mar 26	Su			–
3	Mar 28	T	II	Electronic structure – theory	
4	Mar 30	R	II	Quantum-Espresso – praxis	
	Apr 2	Su			Quiz 1 Project 1
5	Apr 4	T	II	Quantum-Espresso – walkthrough	
6	Apr 6	R	II	Quantum-Espresso – walkthrough/project	
	Apr 9	Su			–
7	Apr 11	T	II	Quantum-Espresso – project	
8	Apr 13	R	III	Molecular dynamics – theory	
	Apr 16	Su			Quiz 2 Project 2
9*	Apr 18	T	III-A	LAMMPS – praxis	
10	Apr 20	R	III-A	LAMMPS – walkthrough	
	Apr 23	Su			–
11	Apr 25	T	III-A	LAMMPS – walkthrough / project	
12	Apr 27	R	III-A	LAMMPS – project	
	Apr 30	Su			Project 3A
13	May 2	T	III-B	Gromacs – praxis	
14	May 4	R	III-B	Gromacs – walkthrough	
	May 7	Su			Term Project Topic
15	May 9	T	III-B	Gromacs – walkthrough / project	

16	May 11	R	III-B	Gromacs – project	
	May 14	Su			Quiz 3 Project 3B
17	May 16	T		Advanced techniques / Term project	
18*	May 18	R		Advanced techniques / Term project	
	May 26	F			Term Project Report

* Prof. Ferguson likely on travel these dates and not available for class / discussion, appropriate arrangements TBA.