JOINT INSTITUTE
交大密西根学院

Course Syllabus

VK 554

Computational Approaches in MSE

2022 Spring

Course Description:

This course provides a comprehensive introduction to the theories and applications of common modeling and simulation techniques in the field of materials science and engineering. Specifically, the course will focus on the basic mathematic and physical theories for density functional theory (DFT), molecular dynamics (MD) and phase field method (PFM), together with their algorithm implementations and practical operations. A few case studies will be conducted, to show the advantages and limitations of the above techniques in solving MSE related problems. In addition, the course will briefly discuss the applications of the emerging artificial intelligence techniques and supercomputers in materials science, demonstrating the design of several machine learning models and the realization of basic parallel computing algorithms.

Instructor:

Name: Yanming Wang
Email: yanming.wang@sjtu.edu.cn
Phone: +86-21-34206765 Ext. 5251
Office: Room: Room 525, Longbin Building
Office hour: TBD

COURSE OBJECTIVES:

1. To teach the basic concepts of quantum mechanics and the density functional theory (DFT).
2. To teach the fundamental principles of classical statistical mechanics and the molecular dynamics (MD) method.
3. To explain the mathematic background and general formulation of a phase field model (PFM).

4. To discuss the connections and differences among the computational methods at different time and length scales.
5. To introduce several common machine learning algorithms and their applications in computational materials science.
6. To introduce the basic concepts and implementation methods for parallel computing.

COURSE OUTCOMES:

After completing this course, students should be able to:

1. Understand the approximations and assumptions of DFT, and perform DFT calculations for material property predictions.
2. Apply MD to investigate dynamical properties of a material system.
3. Develop a basic phase field model for investigating phase transition and interface related problems.
4. Distinguish the application areas and conditions of different simulation and modeling techniques, and propose possible computational approaches to a given materials science problem.
5. Know commonly used machine learning models for materials design and property prediction.
6. Clarify the hardware and software requirements for performing large-scale simulations, and understand basic parallel computing algorithms.

Textbook (Author, Book Title, Publisher, Publication Year, ISBN)**:**

1. Slides used in the lectures.
2. Marques, Miguel AL, and E. K. U. Gross. "A primer in density functional theory." Lecture Notes in Physics 620 (2003): 144-184. (Suggested reading)
3. Daan Frenkel and Berend Smit. Understanding Molecular Simulation: From Algorithms to Applications, 2nd Edition, Elsevier, 2002. (Suggested reading)
4. Biner, S. Bulent. Programming phase-field modeling. Switzerland: Springer International Publishing (2017). (Suggested reading)

Course Prerequisites:

Fundamentals of materials science; Basic knowledge of computer programming.

Course Website:

TBD.

Grading Policy (Assignments %, Project, Exams, etc.)**:**

Homework	40%
Project	40%
Final Exam	20%
Total	**100%**

Honor Code Policy:

- **Honor Code:** All students in the class are bound by the Honor Code of the Joint Institute (https://www.ji.sjtu.edu.cn/academics/academic-integrity/honor-code/) as well as the ***Addendum to the Honor Code for Online Teaching***. You may not seek to gain an unfair advantage over your fellow students; you may not consult, look at, or possess the unpublished work of another without their permission; and you must appropriately acknowledge your use of another's work.
- Attendance: Attendance to the lectures is strongly encouraged. On-line attendance is acceptable under the conditions when difficulties exist for in-person attendance. Reasonable explanations need to be given for continuous absence for more than *one week*.
- Participation: Active participation is highly expected for all students, including interactive activities during the lecture, attendance of instructor's office hours, in-person and on-line discussions with instructor and other students in a proper way, etc.
- Assignments: Unless specified, all the assignments are *individual* assignments, and all submissions must represent the student's own work. Duplicated submission is not allowed and will trigger an honor code violation investigation. However, students are encouraged to discuss course topics and help each other to understand the problems.
- Submission: All assignments should be submitted electronically on Canvas before the specific deadline.
- Exams: Exams will be conducted following all the standard regulations of JI and SJTU. If needed, additional procedures will be announced prior to the exams. Anyone who fail to follow the procedures will be given an 'F' for the exam.

Addendum to the Honor Code for Online Teaching

- The Honor Code in the Context of Online Courses

The JI Honor Code applies to courses taught in an online fashion in the same way that it does to all courses. It is worth repeating the central tenets here:

- Engineers must possess personal integrity as students and as professionals. They must honorably ensure safety, health, fairness, and the proper use of available resources in their undertakings.

- Members of JI are honorable and trustworthy persons.
- The students, faculty members, and staff members of JI trust each other to uphold the principles of the Honor Code. They are jointly responsible for precautions against violations of its policies.
- It is dishonorable for students to receive credit for work that is not the result of their own efforts.

In particular, the parts of the Honor Code regarding conduct during in-class examinations, for coursework, projects etc. apply correspondingly for such work conducted in courses taught online. Additional rules adapted to remote examinations, coursework etc. may be imposed as necessary.

In addition, students are required to abide by following rules specific to online teaching. These requirements are provisionally considered part of the Honor Code for the current teaching term.

Due to the new types of interaction and the new forms of learning activities there may be further issues that are not covered below. Students should not hesitate to contact their instructor, the Honor Council (jihonor@sjtu.edu.cn) or the FCD (jifcd@sjtu.edu.cn) if they have any questions.

- Online Presence and Activities

The Joint Institute imposes a “real name” policy for all online activities organized by JI instructors. This policy applies to groups or communication by E-Mail, Canvas, Piazza, Feishu, WeChat and all other platforms where groups are set up by JI or by individual instructors for students attending JI courses, events or other activities.

Students are required to use their actual name (in Pinyin) as part of their online presence for such groups and when communicating online. Individual instructors may also require students to add their name in Chinese characters (if applicable) and/or their Student ID.

Unless otherwise noted, such online activities are intended for the exclusive participation of JI students. Account names, meeting IDs, passwords and other information intended to protect the exclusivity of such activities may not be shared with anyone who is not part of the course or activity.

For example, it is not permissible to give a Feishu meeting ID of a given course to any person who is not enrolled in that course, whether or not the person is a JI student.

- Online Etiquette

When communicating or otherwise using online groups, students should follow the regulations set down by instructors concerning the use of online tools. Vandalism, spam messages, verbal and other forms of abuse, violation of English-only policies (as detailed by instructors) and disturbance of the learning experience of other students are not permitted.

- Teaching and Learning Materials

Teaching and learning materials, such as lecture slides, assignments, quizzes, videos etc. are copyrighted and may not be passed on to others without the express permission of the course instructor. This applies in particular to recordings of Zoom lectures and other videos created by instructors.

In particular, it is not permissible to upload videos to sharing platforms (such as Youku or YouTube) or to post lecture slides, assignment questions, project descriptions etc. on public sites such as

SlideShare.

Course Assessment Methods:
Homework:
Homework problems are designed such that the students can apply and exercise the knowledge taught in the lectures. Through solving these problems, the students are expected to better understand the underlying theories and algorithms in the field of computational materials science.

Project:
Group (or individual) project(s) is (are) assigned to the students, to practice their skills of simulations and modeling for solving problems in the area of materials science. The students may choose the topics that are relevant to their own research. Typically, an in-class presentation and a written report (with attaching the code and script if applicable) are required as proof of the accomplishment of the project.

Examination:
Final exam is a means to comprehensively measure the students' level of achievement of the Course Outcomes. Typical types of exam problems may include T/F and multiple-choice questions, proofs, derivations, calculations, sketches, and etc. If the form of the examinations is determined to be on-line, then the submission is expected to be via Canvas and handing in the exam papers in person is not accepted.

Teaching Schedule:

Week	NO.	lectures and Exams	Comments
1	1	Course introduction and an overview of computational materials science	
	2	Relevant materials science background knowledge; Basic Linux operations and algorithms I	
2	3	A short intro to quantum mechanics	
	4	Density functional theory I; Basic Linux operations and algorithms II	
3	5	Density functional theory II	
	6	Applications of DFT and case studies	
4	7	A short intro to statistical mechanics	
	8	Molecular dynamics I; Molecular dynamics II	
5	9	Molecular dynamics III	
	10	Applications of MD and case studies	

6	11	Phase field method I	
	12	Phase field method II; Applications of PFM and case studies	
7	13	Other common computational models	
	14	Multi-scale modeling approaches and case studies	
8	15	-	Tomb sweeping day
	16	Machine learning for materials science; Computation-based materials design	
9	17	Parallel computing techniques I	
	18	Parallel computing techniques II	Potentially a visit to the SJTU HPC center
10	19	Project presentations	
	20	Final exam (Tentative)	