CHE 478/578: Introduction to Molecular Simulation

Spring 2017

Tueday and Thursday: 4:30 – 5:45 pm (FH 267)

Elective course

Catalog description: CHE 478/578 Introduction to Molecular Simulation
Prerequisites (by topic): *Solid knowledge of chemical engineering thermodynamics, knowledge of classical mechanics on an introductory level, knowledge of multivariable integral and differential calculus, knowledge of basic statistics, knowledge of some higher programming language.*
Connection between mechanics and thermodynamics, statistical mechanics. Intermolecular forces. Basic principles, molecular dynamics and Monte Carlo simulation. Corresponding states and phase equilibrium from molecular simulation. Optional special topics. Examples of computer codes.

Textbook: None, part of instructor's lecture notes will be made available to students.

References: A list of recommended further readings will be provided and put on reserve in the library for the class period.

Coordinator: Dr.-Ing. habil. Rolf Lustig
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Office Hours: TTh 3 – 4 pm (or by appointment)

Course objectives:
Molecular simulation is a way to predict thermophysical properties from scratch. The only input to this concept are the forces acting between the individual atoms or molecules making up the system. This method is extremely demanding computationally, and has evolved from being an academic luxury to being a practical tool in engineering due to the dramatic developments in low-cost computer hardware technology. Most if not all major companies in the chemical industry have established or are establishing research labs in molecular simulation. Software companies are founded to commercialize these methods. The discipline is comprised of: Classical mechanics, thermodynamics, and statistical mechanics as the connecting piece. The course reviews the underlying physical principles and focuses on applications.

This course is designed to:
1. Have students develop an appreciation for the molecular origin of macroscopic phenomena.
2. Provide students with skills to set up basic simulation programs on their own.
3. Emphasize accuracy and efficiency concepts and their relation to the algorithm selection process.
4. Provide students with a critical understanding of the capability of commercial software packages.

Expected Outcomes: Upon successful completion of this course, students should be able to:
1. Understand macroscopic phenomena in terms of intermolecular interactions.
2. Formulate and analyze specific thermophysical problems using molecular concepts.
3. Identify an appropriate simulation technique for the treatment of a given thermophysical problem.
4. Understand the implications of algorithm selection on the accuracy and efficiency of numerical results.
5. Write and modify computer programs for the prediction and interpretation of thermophysical properties.

Fulfills Program Outcomes:
- a) Ability to apply Mathematics, Science, and Engineering knowledge.
- e) Identification, formulation, and solution of Engineering problems.
- j) Use techniques, skills, and modern engineering tools necessary for Engineering practice.
- k) Principles and working knowledge as defined by AIChE program criteria.

Topics:

The following is a tentative list of topics, which the instructor intends to cover in this course. The amount, sequence, and depth of the material will depend on the background and interests of the students.

- Introduction
- Structure of classical mechanics, thermodynamics, and statistical mechanics
- Intermolecular forces
- Basic principles of molecular simulation
- Molecular dynamics simulation
- Monte Carlo simulation
- On the significance of the theorem of corresponding states
- Phase equilibrium from molecular simulation
- Special topics (optional, i.e. mixtures, chemical reactions, transport properties)
- Examples

Organization:

The course will be taught on the graduate level, irrespective the relative numbers of undergraduate and graduate students enrolled.

Since the logical basics of this course are abstract and progressive, attendance to lectures is mandatory for successful completion. If a class is missed, the student is responsible for the covered material. There will be no traditional homework assignments. However, depending on available time and class size, a project may be assigned, and the students may be asked to present their findings in front of the class. The instructor will initiate frequent discussions about the covered material to invoke student feedback. Such contributions will constitute part of the grade. Exams will focus on basic understanding and technical communication rather than formalities. There will be a midterm exam after about half of the course and a final exam on the day scheduled by the administration. Both exams may take on the form of a project. Be advised that the instructor will pay close attention to possible duplication and plagiarism issues.

CHE 478:

Undergraduate students are expected to master the material as delivered in the lectures and class discussions. Theoretical background and necessary simulation techniques for projects and exams will be thoroughly discussed in class.

CHE 578:

Graduate students are expected to demonstrate an ability to expand on the material as delivered in the lectures and class discussions by performing in-depth literature studies to be announced. The instructor will be available for advice and supervision beyond class time.

Grading:

Projects and participation:	30%
Midterm exam:	30%
Final exam:	40%

Prepared by: Rolf Lustig, January 2017