CHM 6580

Special Topics in Physical Chemistry

Force Field Development and Applications

Instructors: Coray Colina, Ping Lin

Fall 2016

Time: Tuesday, Wednesday: Periods 3, 4

Location: CBL 313

Textbooks:

A.R. Leach, "Molecular Modeling: Principles and Applications", 2nd edition, Prentice-Hall, ISBN 0-582-38210-6 (2001)

Instructors:

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Office hours:

Wednesday 11:30 am to 12:30 pm, or upon request (send email to the instructors).

Course Description:

Current methods for modeling soft matter at the atomistic or coarse-grained levels rely significantly on the empirical potential energy function (i.e. "force fields") selected to calculate energies and forces that determine configurations and dynamics. However, representing complex interactions using computationally available functional forms remains a challenge. This course will present an overview of popular force fields, and discuss their development philosophy and applications. Some in-depth discussion will be provided for AMBER, TraPPE, GAFF, CGenFF, and PCFF. Comparison of their performances on specific applications will also be given, as well as an introduction to force field development for new molecules for particular applications. At the conclusion of the course, students will understand the physical basis and philosophy behind the force fields mentioned above, and their proper usage.

Course Objectives:

1. To provide students with a general overview of popular force fields in modeling soft matter, nano-materials and biomolecular systems, including additive MM force fields - Class I and II, polarizable force fields, reactive force field, coarse-grained force field.

2. To provide students with an in depth knowledge of class I force fields, including the development of the AMBER force field for molecular dynamics simulation to appreciate and understand the use of it in research of biomolecular systems and soft matter, including polymers.

3. To provide students with an in depth knowledge of class II force fields, including the development of the PCFF force field for molecular dynamics simulation to appreciate and understand the use of it in research of polymeric systems.

4. To provide students with the background and skills needed to read the force field simulation literature and evaluate it critically.

5. To teach students basic aspects in generation and assignment of force field parameters for a new molecule using Antechamber and GAFF.

6. To provide students with an in depth knowledge of Coarse Grain potentials, including coarse-grain TraPPE.

7. To teach students how the above material is related, so that they can make predictions for applications to fluids, interfaces, polymers, surfactants, colloids, nanostructured materials and biological systems.

The specific topics to be covered include:

A. A general overview of popular force fields in modeling soft matter, nano-materials and biomolecular systems, including additive MM force fields - Class I and II, polarizable force fields, reactive force field, coarse-grained force field. (1 week)
B. The development of the AMBER force field for molecular dynamics simulation of biomolecular systems. (2 weeks)
C. The Transferable Potential for Phase Equilibria (TraPPE) family of force fields for modeling complex chemical systems. (2 weeks)
D. Parameterization process in general AMBER force field (GAFF) for rational drug design. (2 weeks)
E. The difference between CHARMM General Force Field (CGenFF) and GAFF. (2 weeks)
F. class II force field: PCFF. A force field developed for polymers and other materials. (1 week)
G. Comparison of AMBER, CHARMM, COMPASS, GROMOS, OPLS, TraPPE and UFF for prediction of vapor-liquid coexistence curves and liquid densities. (1 week)
H. How to generate and assign force field parameters for a new molecule using Antechamber and GAFF. (1 week)
I. Reparameterization of GAFF for small solutes with an emphasis on free energies of hydration. (1 week)

J. An example of coarse-graining method and force field development. (1 week)
K. Applications of force fields by examples. (2 weeks)
Requirements. This course is suitable for graduate students looking forward to getting in-depth information about force fields and its development and application. A graduate level molecular simulations course is required as a pre-requisite (*e.g.* CHM 6586.)

Course Organization and Grading.
The course material will be covered in 2 sessions per week.

Assessment Tools

1. Problem sets and homework that allow student collaboration and team-work.

2. Individual Projects.

"Requirements for class attendance and make-up exams, assignments, and other work in this course are consistent with university policies that can be found at:

https://catalog.ufl.edu/ugrad/current/regulations/info/attendance.aspx."

Information on current UF grading policies for assigning grade points can be found at:

https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx.

Academic Integrity

All University policies regarding academic integrity/academic dishonesty apply to this course and the students enrolled in this course. Team-work is encouraged provided that each team is comprised by 2 (max) people and the instructors are notified by email before each homework is started; otherwise, each student in this course is expected to work entirely on her/his own while taking any assessment without the assistance of others, and to abide by University policies about academic integrity and academic dishonesty. Academic dishonesty can result in assignment of "F" by the course instructors or "XF" by Judicial Affairs as the final grade for the student.

Academic dishonesty is not limited to simply cheating on an exam or assignment.

Academic dishonesty includes, but is not limited to, cheating, plagiarizing, fabricating of information or citations, facilitating acts of academic dishonesty by others, having unauthorized possession of examinations, submitting work of another person or work previously used without informing the instructor, or tampering with the academic work of other students.

Remember that "UF students are bound by The Honor Pledge which states, "We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest

standards of honor and integrity by abiding by the Honor Code. On all work submitted for credit by students at the University of Florida, the following pledge is either required or implied: "On my honor, I have neither given nor received unauthorized aid in doing this assignment." The Honor Code (http://www.dso.ufl.edu/sccr/process/student-conduct-honor- code/) specifies a number of behaviors that are in violation of this code and the possible sanctions. Furthermore, you are obligated to report any condition that facilitates academic misconduct to appropriate personnel. If you have any questions or concerns, please consult with the instructor or TAs in this class."

In addition, any attempt to hack the homework server, any incidents of coping, saving, and/or transmitting materials from the on-line laboratories, and any attempts to tamper with the grades on elearning/CANVAS or the homework-server will be prosecuted though the academic integrity channels.

In addition, any attempt to hack the quiz server, any incidents of coping, saving, and/or transmitting materials from the on-line quizzes and homeworks, and any attempts to tamper with the grades on elearning/CANVAS or the quiz-server will be prosecuted though the academic integrity channels. The University and College guidelines can be found at the College Academic Integrity web site:

Accommodations for students with disabilities

The Office of Disability Services (www.dso.ufl.edu/dcr) requests and maintains disability-related documents; certifies eligibility for services; determines academic adjustments, auxiliary aids, and/or services; and develops plans for the provision of academic adjustments, auxiliary aids, and/or services.

"Students with disabilities requesting accommodations should first register with the Disability Resource Center (352-392-8565, www.dso.ufl.edu/drc/) by providing appropriate documentation. Once registered, students will receive an accommodation letter which must be presented to the instructor when requesting accommodation. Students with disabilities should follow this procedure as early as possible in the semester."

Online course evaluation process

"Students are expected to provide feedback on the quality of instruction in this course by completing online evaluations at https://evaluations.ufl.edu. Evaluations are typically open during the last two or three weeks of the semester, but students will be given specific times when they are open. Summary results of these assessments are available to students at https://evaluations.ufl.edu/results/."

Additional Information

Contact information for the Counseling and Wellness Center:
http://www.counseling.ufl.edu/cwc/Default.aspx, 392-1575; and the University Police Department: 392-1111 or 9-1-1 for emergencies.