Special topics: Statistical Mechanics applied to Molecular Simulations

Course Information

Course number: CHM 6580
Course title: Special Topics**Credits:** 3
Where: Room WEIL 0408D.
When: Tuesdays (periods 2,3 (8:30-10:25) and Thursdays 3 (9:30 am –10:25am)
Classes start/end: 8/24/21 - 12/7/21
No class on Sep 5th and Nov 23th

List of Recommended Textbooks:
Dan Zuckerman, "**Statistical Physics of Biomolecules: An Introduction".** This is one of my all-time favorites. If you are serious about stat mech, you should read this book.

Mark Tuckerman, "Statistical Mechanics: Theory and Molecular Simulation".

Ken Dill and Sarina Bromberg. "Molecular Driving Forces". Ken has a special ability to make hard problems seem easy. He changed how I look at research, and his book changed how I write, and present research. There are beautiful illustrations of the different concepts through out the book made by Sarina and plenty of short exercises to help you solidify concepts. If you only had one book about stat mech … I would recommend this one! Like in many enhanced sampling approaches—I might be biased!

Christop Schüte and Marco Sarich, "Metastability and Markov State Models in Molecular Dynamics". Published by the American Mathematical Society and Courant Institute of Mathematical Sciences, this book has quite a bit of Math – but so do many of the MSM papers in this field. I will rely on this book even though it is often beyond my comfort zone – my goal would be that when you read papers from our field on MSM you don't gloss over the equations and can actually follow what they are doing and why.

Greg Bowman, Vijay Pande, Frank Noe, "An introduction to MSM and Their Application to Long Timescale Molecular Simulation". This is a book by articles – you can download most of the articles through UF's library system as regular articles. This is a rapidly developing field, so some of the issues presented here (2014) might already have solution – but the foundation they provide is invaluable.

Lau, Dill, 1989. "A Lattice Statistical Mechanics Model of the Conformational Sequence Spaces of Proteins". Macromolecules, 22, 3986-3997. This an other papers on the HP lattice model will be valuable to our discussions on HP lattice Models

Tools

Prody (http://prody.csb.pitt.edu/)

HP Sandbox (https://github.com/vvoelz/HPSandbox)

Cpptraj

Course Description: We will cover three basic blocks:

-Essential Dynamics, quasiharmonic analysis, Schiltter and Andricioaei's entropy. Interpretation of eigenvectors and eigenvalues, comparison of ensembles, collectivity measures

-HP lattice models: a case study for systems where we can obtain the partitition function.

-MSMs: derivation, application, benefits, challenges. Dynamical Graphical Models, Decomposable Markov State Models.

The dynamics of the class will include formal explanations, guided activities, and student guided literature discussion and final projects involving a presentation and written work.

Online material: Available through canvas (https://elearning.ufl.edu/)
It will contain the syllabus, and lecture notes. It will also serve as a mode of email communication (you can configure it to redirect the emails).

Instructor Information

Alberto Perez
Assistant Professor
Office: Room 240F Leigh Hall.
Office hours: By appointment.
Contact e-mail: perez@chem.ufl.edu

Face to face learning

Attendance: Attendance to lectures is expected as this is a computational lab. We will combine a traditional lecture with application problems. In addition to the 3 hrs class a week, ~8-10/week of reading, homework and general study are required.

Homework and Grading

Homework: There will be coursework that will not be graded but will benefit assimilation of concepts

Final Projects: There will be two groups each preparing a different topic as a final project.
Project 1: Dynamical Graphical Models

Project 2: Decomposable Markov State Models

A written document and presentation will be evaluated. The presentation will include two parts: 1) a discussion on recent literature, a perspective on the current application, the limitations and challenges ahead. An demo application performed by the team would be strongly encouraged.

Class discussions: there will be three graded literature discussions in class.

Course Grading: The grade will be determined by discussion (30%), final project document (25%), presentations (25%) and in-class participation (20%).

There is NO FINAL in this class.

Course Evaluations: 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/.

HONOR CODE The student honor code can be found at http://www.registrar.ufl.edu/catalog/policies/students.html

The students, instructor and TAs are honor bound to comply with the Honors Pledge:

We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honesty and integrity.
On all work submitted for credit by students at the university, the following pledge is either required or implied: On my honor, I have neither given nor received unauthorized aid in doing this assignment.

Cheating on an exam will result in a grade of zero. Although homework is expected to be worked "in group", the submitted homework solution must be your individual work. If any homework or quiz assignment is suspect, a grade of zero will also be given for that assignment.

Information on current UF grading policies for assigning grade points is available at https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx

Students with disabilities: Students requiring special accommodations need to register at the Dean of Student Offices and bring the documentation to the instructor.

Counseling services are available at **http://www.counsel.ufl.edu .** or call (352)-392-1575 during regular service hours (8am-5pm). For other hours or weekends call the Alachua County Crisis Center (264-6789). Students may also call the clinician on-call at Student Mental Health for phone callback and consultation at (352)-392-1171.

Campus Resources:

Health and Wellness
U Matter, We Care: If you or someone you know is in distress, please contact umatter@ufl.edu, 352-392-1575, or visit U Matter, We Care website to refer or report a concern and a team member will reach out to the student in distress.
Counseling and Wellness Center: Visit the Counseling and Wellness Center website or call 352-392-1575 for information on crisis services as well as non-crisis services.
Student Health Care Center: Call 352-392-1161 for 24/7 information to help you find the care you need, or visit the Student Health Care Center website.
University Police Department: Visit UF Police Department website or call 352-392-1111 (or 9-1-1 for emergencies).
UF Health Shands Emergency Room / Trauma Center: For immediate medical care call 352-733-0111 or go to the emergency room at 1515 SW Archer Road,
Gainesville, FL 32608; Visit the UF Health Emergency Room and Trauma Center website.

Academic Resources

E-learning technical support: Contact the UF Computing Help Desk at 352-392-4357 or via e-mail at helpdesk@ufl.edu.
Career Connections Center: Reitz Union Suite 1300, 352-392-1601. Career assistance and counseling services.
Library Support: Various ways to receive assistance with respect to using the libraries or finding resources.
Teaching Center: Broward Hall, 352-392-2010 or to make an appointment 352- 392-6420. General study skills and tutoring.
Writing Studio: 2215 Turlington Hall*,* 352-846-1138. Help brainstorming, formatting, and writing papers.
Student Complaints On-Campus: Visit the Student Honor Code and Student Conduct Code webpage for more information.
On-Line Students Complaints: View the Distance Learning Student Complaint Process.

Course Objectives

By the end of this course students should be able to:

1. Understand when, which and how to use computational tools to gain insights into chemical systems.
2. Gain a basic understanding of how to run quantum mechanical calculations on small molecules.
    a. Base superposition error
    b. Counterpoise method
3. Gain a basic understanding of how to use classical mechanics tools for the simulating larger biomolecules.
4. An introduction to software packages for computational chemistry
5. Model building and molecular mechanics

6. Molecular orbitals and electronic structure
7. Solvation effects and molecular dynamics
8. Building large systems (polymers and solid surfaces)

Suggested Course itinerary:

Date	Topics
Jan 10th	Introduction, class dynamics, Literarture for first discussion
Jan 12th	Incomplete sampling, ensemble comparison
Jan 17th	Essential dynamics, quasiharmonic analysis, matrices
Jan 19th	Essential dynamics, quasiharmonic analysis, matrices II
Jan 24th	Literature discussion I (graded)
Jan 26th	HP lattice models, literature for second discussion
Jan 31st	HP Sampling MC, REMC vs exact solution.
Feb 2nd	Biased MC, effects of ambiguous data
Feb 7th	Literature discussion II (graded)
Feb 9th	Introduction to MSMs, literature list for third discussion
Feb 14th	Pyemma Pentapeptide walkthrough
Feb 16th	Literature review MSM I
Feb 21st	Literarture review MSM II
Feb 23rd	Purushottam Dixit (physics) lecture on MSM
Feb 28th	Transfer Operators, projection
March 2nd	Aib Peptide
Marh 7 th	FAST method / methods for seeding MSMs
March 9th	Biases in MSMs
March 14	Spring Break, no class
March 16th	Spring Break, no class
March 21st	Limitations of MSMs
March 23rd	(Invited presentation at Temple University)
March 28th	Presentation group 1
March 30th	The bigger picture: allostery, epigenetic changes, post-translational modifications,…
April 4th	Presentation group 2
April 6th	Transition path theory
April 11th	Role of machine learning in MSMs

April 13th	Designing toy models
April 18th	Literature discussion III (graded)
April 29th	Literature discussion III (graded)
April 25th	Closing Remarks

Grading scale:

A > 90
A- 87.5 to 89.99
B+ 82.5 to 87.49
B 77.5 to 82.49
B- 75 to 77.49
C+ 72.5 to 74.99
C 67.5 to 72.49
C- 65 to 67.49
D+ 62.5 to 64.99
D 57.5 to 62.49
D- 55 to 57.49
E <60

Grade Values for Conversion

Grades	Grade Points		
A	4.0	D+	1.33
A-	3.67	D	1.0
B+	3.33	D-	.67
B	3.0	E	0
B-	2.67	WF	0
C+	2.33	I	0
C	2.0	NG	0
C-	1.67	S/U	0