Computational Biophysics

Intructor: Prof. Luis Cruz Cruz
Lectures: Tuesdays, Thursdays 11:00 am – 12:20 pm, Disque 919
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A) Course Description

This course is the combined graduate and undergraduate topical course of computational biophysics provided by the Department of Physics. This course will cover the theory and application of molecular simulations to problems in biological physics. Using classical and statistical mechanics, we will cover topics including atomic scale simulations, statistical sampling, error analysis, and models of proteins and their dynamics in model cellular environments. Additionally, the course will present topics from Computational Neuroscience. This course is an exploratory course in the sense that it will not provide expertise in any one area of computation but will provide students with a general view of the theory and available tools that can be applied to general molecular biophysical problems and neural networks. This course meets the needs of those wanting an introduction to computational biophysics. At the same time, it also meets the needs of those already familiar with the tools but that want to know the inner workings and theoretical background.

B) Organization

Although this course will be presented in a lecture-based format, there will also be computer demonstrations as some of the topics are best *demonstrated* rather than *stated*. However, this will not be a "passive" course in the sense that students (you!) are expected and will be required to participate during class – this is not an option and will count towards the final grade. The side effects of participation is that everyone will benefit from questions and answers and will also provide you with the ability to "slow down" the lecture and go over topics that would otherwise go unclear.

There will be a midterm and a final, regular homework assignments, and a final project. Homework may consist of mathematical derivations, concept investigations, problem solving, and/or computer investigations. To gain the most of this course, you should be familiar with a computer language as the computer investigations may require some amount of coding and/or interaction with computers. Access to computers and computational tools will be disclosed as they become available during the course, but computations in general will not require more than the processing power provided by modern laptops.

C) Course Objectives

After completing this course, students should be able to:

- Articulate an understanding of the general focus of computational biophysics and illustrate with particular molecular examples.
- Interpret biophysical phenomena in terms of the underlying atomic processes and their governing laws of classical and statistical mechanics.
- Recall and explain the underlying theory behind computational biophysics.
- Describe different computational approaches and their strengths and weaknesses.
- Analyze complex protein dynamics and interactions in terms of simple mathematical models.
- Calculate statistical analysis and perform error analysis of correlated data.
- Use standard computational packages to tackle problems in biophysics.
- Design and code appropriate computer algorithms to compute biophysical quantities that can be compared with experimental results.

This course will meet the following Drexel's Learning Priorities:

- Creative And Critical Thinking: by using convergent thinking (critical thinking, evaluation of ideas, quantitative/qualitative analysis, scientific reasoning) to generate novel and relevant ideas, strategies, approaches, or products.
- Information Literacy: by using skills and knowledge to access, evaluate and use information effectively, competently, and creatively.
- Technology Use: by using appropriate technologies to communicate, collaborate, solve problems, make decisions, and conduct research, as well as foster creativity and life-long learning.

D) Tentative Course Schedule

The course will cover the following list of topics in the following tentative schedule:

Week	Lecture	Date	Topics	Hmwrk Due
1	1	Jan 05	Introduction; Atomic Systems; Molecular Systems	
	2	Jan 07	Equations of Motion; Hamilton Dynamics; Finite Difference Methods	
2	3	Jan 12	Constraint Dynamics; Checks on Accuracy; Hard Spheres; Thermodynamics and Structural Properties	
	4	Jan 14	Transport coefficients; Error analysis; Boundary Conditions	**1**
3	5	Jan 19	Initial Conditions; Equilibration; Energy Minimization	
	6	Jan 21	Steepest Descent; Conjugate Gradient	**2**
4	7	Jan 26	"Tricks" of the Trade	
	8	Jan 28	Neighbor Lists; Multiple Time Steps; Ewald Sum	**3**
5	9	Feb 02	Mean Field Approximation; Dimensionless Units	
	Midterm	Feb 04		**4**
6	10	Feb 09	Step-wise Potentials	
	11	Feb 11	Langevin's Dynamics	**5**

7	12	Feb 16	Monte Carlo Dynamics; Metropolis Algorithm	
	13	Feb 18	Thermodynamic Ensembles	**6**
8	14	Feb 23	Molecular Liquids; Liquid Crystals	
	15	Feb 25	Polymers; Conformations of Ideal Chains; Radius of Gyration	**7**
9	16	Mar 01	Motion of Polymers; Molecular Dynamics	
	17	Mar 03	Motion of Bonds, bending; Dihedral Motion; Non-bonded energy terms; Force Fields; Models for Water	**8**
10	18	Mar 08	Protein Structure; Conformational Analysis; Comparative Modeling; Models for Folding and Unfolding	
	19	Mar 10	Brief Introduction to the biology and applications of Neural Networks	**9**
	FINAL	**TBA**		**Final Project**

E) Textbooks

The recommended textbook for the course is reference 1 listed below. However, the complete sources for the presented material are varied and will include the lecture slides, notes, and other reproduced material from various other sources that will be provided as the course progresses. The other main textbooks on which this course is based are listed below. I recommend that you check their availability in the library as they could be of use as supplementary references. The reference books are:

1. *Understanding Molecular Simulation: From Algorithms to Applications*, D. Frenkel and B. Smit, Academic Press, 2nd Edition, ISBN: 978-0-12-267351-1.
2. *Computer Simulation of Liquids*, M. P. Allen and D. J. Tildesley, Oxford.
3. *Molecular Modelling: Principles and Applications*, A. R. Leach, Prentice Hall.
4. *Molecular Modeling and Simulation: An Interdisciplinary Guide*, T. Schlick, Springer.
5. *The Art of Molecular Dynamics Simulation*, D. C. Rapaport, Cambridge University Press.
6. *Molecular Modelling for Beginners*, A. Hinchliffe, Wiley.
7. *Molecular Dynamics Simulation: Elementary Methods*, J. M. Haile, Wiley.
8. *Polymer Physics*, M. Rubinstein and R. H. Colby, Oxford.
9. *Fundamentals of Computational Neuroscience,* T. P. Trappenberg, Oxford.
10. *Neural Network Design, 2nd Edition,* M.T. Hagan, H.B. Demuth, M.H. Beale, O. De Jesús

F) Grading

The final course grade will be based on the following weights:

Midterm	12 %
Final	13 %
Homework	40 %
Attendance/Participation	10 %
Final Project	25 %

TOTAL	100 %

The grading scale in percentages is as follows.

A+ ≥ 97	B+ = 87-89	C+ = 77-79	D+ = 67-69
A = 93-96	B = 83-86	C = 73-76	D = 60-66
A- = 90-92	B- = 80-82	C- = 70-72	F ≤ 59

1. **MIDTERM:** A midterm will be given on week 5. There is **no make-up for the midterm**. If you miss the midterm and have a documented, valid reason for doing so, please discuss it with the course director as soon as possible.
2. **HOMEWORK:** Regular homework will be assigned and be due on the date specified above, usually one week after the day they are handed out. All homework must be submitted by their due dates. Late submissions will be subject to a 10% reduced credit *per late day;* however students are expected to turn in all homework (even if late).

   Work in groups is encouraged, but the submitted homework is individual and cannot be shared or "signed" by more than one person. Duplicates or works that look very similar to each other will not be graded for either party. In other words, the homework has to be a personal product of your own work.
3. **ATTENDANCE AND PARTICIPATION:** Attendance to lecture is required. Excuses are accepted, but they have to be disclosed before lecture. Other absences are only excused with proper medical documentation. Participation is part of the course and the course director reserves the right to elicit comments, questions, or comments related to the course from any of the students attending the course.
4. **FINAL EXAM:** The final exam is comprehensive – it will be based on all the subject material covered in the course.
5. **FINAL PROJECT:** The final project will consist of readings of papers from the literature and/or the completion of a numerical investigation.
6. **CLASSROOM RULES OF CONDUCT:** In general, any electronic or mechanical equipment, any material, books, or literature unrelated to the course and/or that may take your attention or that of your classmates away from class discussion are strictly prohibited. Being the content of the course heavy on concepts and phenomena, it is expected that you will dedicate all your attention and focus to the topic under discussion. Please note that this particularly applies to the restriction in the use of laptops during lecture (i.e. strongly discouraged). Behavior that is not considered constructive to your learning or that may be disruptive to other students will not be tolerated.
7. **ACADEMIC HONESTY:** You may not copy one another's exams or homeworks. These are considered cheating and will be dealt with in the following manner. The first infraction will result in a zero for all parties involved. The second infraction will result in an F for the course and a report to the office of academic affairs.

Drexel's Policy on Academic Honesty can be found online at
http://www.drexel.edu/provost/policies/academic_dishonesty.asp

Consequences of violations of the academic honesty policy can be found at
http://www.drexel.edu/studentlife/judicial/honesty.html

Also review information at
http://www.drexel.edu/studentlife/community_standards/studentHandbook/general_information/code_of_conduct/

Course Drop Policy
http://www.drexel.edu/provost/policies/course_drop.asp

8. **DISABILITY POLICY:** Please let the course instructor know if you have a disability need that has been registered with the Office of Disability Services.

Note: All reasonable attempts will be made to adhere to the schedule and information in this syllabus. However, the instructor reserves the right to make accommodations and adaptations based on class progress, special opportunities, as well as occurrences outside the instructor's control.