TEXAS A&M UNIVERSITY

SYLLABUS

Course title and number	ECEN489/689 Special Topics in Algorithms in Structural Bioinformatics
Term	Spring 2016
Meeting times & location	MW 2:00-3:15pm ENPH 216

Course Description and Prerequisites

This course introduces fundamental concepts, modeling techniques, and computational algorithms in structural bioinformatics especially for students interested in algorithmic development and application for computational challenges arising from the field. With a focus on algorithms involving molecular modeling, systems simulation, optimization, and learning, the course provides essential knowledge for students without prior background in the application domain and addresses learning barriers for them to make unique contributions to the field.

Applications of these algorithms are centered on how to analyze, predict, and engineer biomolecules and biomolecular systems: protein structure and function prediction, molecular dynamics simulation, protein docking, computer-aided drug design, and biomolecular systems engineering. Algorithmic solutions to these applications can provide case studies for algorithmic thinking and innovation. Students interested in practical problem-solving skills for specific applications are also welcome.

The course will involve literature-based presentation, case studies, short projects in homework, and a main final project, in addition to regular lectures.

Prerequisites: Basic knowledge in algorithms and programming. No prior knowledge in biomolecules or biomolecular systems is required.

Learning Outcomes

By taking the course, students are expected

1. to gain knowledge about fundamental concepts, pressing challenges, and rich opportunities in developing and applying algorithms for structural bioinformatics and healthcare;
2. to apply and to strengthen engineering principles and algorithmic thinking to the emerging applications of structural bioinformatics and other fields; and
3. to develop practical skills in computational approaches to analyze, predict, and engineer biomolecules and biomolecular systems.

Instructor Information

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Textbook and Resource Material

Recommended Textbooks:

- **[S]** T Schlick. *Molecular Modeling and Simulation: An Interdisciplinary Guide*. Springer. 2010.
- **[GB]** J Gu and PE Bourne. *Structural Bioinformatics*. Wiley-Blackwell. 2009.

Other References:

- **[D]** B Donald. *Algorithms in Structural Molecular Biology*. MIT Press. 2011.
- **[B]** FJ Burkowski. *Structural Bioinformatics: An Algorithmic Approach.* CRC. 2008.

Additional materials such as tutorials, papers and book chapters will be indicated in class.

Grading Policies

Weights towards final grades for undergraduate students

- 30% Homework
- 30% Midterm Exam
- 40% Final Project Report and Presentation

Weights towards final grades for graduate students

- 20% Homework
- 25% Midterm Exam
- 15% Mini Project
- 40% Final Project Report and Presentation

Tentative Grading Scale:

A	[90%, 100%]
B	[80%, 90%)
C	[70%, 80%)
D	[60%, 70%)
F	[0%, 60%)

Final grades will be determined numerically based solely on individual standing to reflect how well students do in homework, exams, and projects. This approach is adopted to ensure at least a fair mechanism to assess how well students learn course materials and accomplish course goals. Meanwhile, diversity in student background (engineering or science) and academic standing (undergraduate or graduate) will be respected and reflected in final project topics.

Course Topics

Here is the tentative course outline with approximately assigned lecture time:

Week	Topic	Related Reading
1-2	Introduction to biomolecules and structural bioinformatics	**GB**1-3, **S**1-4
2	Molecular visualization	**GB**9
2-3	Protein structure prediction: template-based homology modeling and threading *(Optimization fundamentals; Convex optimization; Sequence alignment as dynamic programming & database search; Threading as linear programming and machine learning)*	**GB**30,31
3-5	Protein structure prediction: ab initio methods *(Structure prediction as energy minimization; Energy function and conformational variables; Nonconvex optimization; Gradient-based and gradient-free algorithms; Ensemble algorithms; Great ideas for objective function, search space and constraints)*	**GB**8,32, **S**8,11,12
5	Molecular dynamics simulation: *Sampling*	**S**13
6-7	Protein flexibility and protein docking *(Dimensionality reduction and optimization algorithms revisited)*	**D**20-23, **GB**24-27
7-9	Protein function prediction from sequence, structure, and big data: *Machine learning*	**GB**21,22
9-10	Computer-aided protein and drug design: *Combinatorial optimization*	**GB**39, **D**11
10-12	Biomolecular system modeling: *Steady states and dynamics*	Literature
13-14	Final project presentation	

Contents may subject to adjustment. Additional research literature will be provided in lectures.

Attendance and Make-up Policies

Regular and punctual attendance to the lectures and recitations facilitates the effective implementation of a systematic study plan. Please consult student rule 7 for additional information: http://student-rules.tamu.edu/rule07.

Americans with Disabilities Act (ADA)

The Americans with Disabilities Act (ADA) is a federal anti-discrimination statute that provides comprehensive civil rights protection for persons with disabilities. Among other things, this legislation requires that all students with disabilities be guaranteed a learning environment that provides for reasonable accommodation of their disabilities. If you believe you have a disability requiring an accommodation, please contact Disability Services, in Cain Hall, Room B118, or call 845-1637. For additional information visit http://disability.tamu.edu

Academic Integrity

For additional information please visit: http://aggiehonor.tamu.edu

"An Aggie does not lie, cheat, or steal, or tolerate those who do."