BE 5320-401 Computational Biophysics
Last updated 12/1/22

Course Number & Title	**Computational Biophysics**	
Credit Units	1 CU (3 semester hours)	
Semester the course will be offered	Spring 2024	
Format e.g. Lecture, Lab, seminar, etc	Lecture	
Class/Laboratory Schedule	2 hrs/week	
Instructor(s)	Gregory R. Bowman	
Cross list, if any	Biochemistry & Molecular Biophysics	
Prerequisites, if any	Admission by permit only, Physical chemistry	
Corequisites, if any		
Course Satisfies	Undergraduate [ ] Mathematics [ ] Natural Science [ ] Core Engineering Requirement [ ] Engineering, technical, non-core [ ] Engineering & Applied Science (EAS)	Graduate [ ] Mathematics [x] Biological Science [x] Bioengineering graduate courses/BE Fundamentals [ ] Other: ______________________
Will this course count as a the Technology in Business and Society Course?	No	
Text(s)/Required Materials		
Catalog Description	This course targets graduate students and upper level undergraduates with adequate background in physical chemistry. Proteins and other biomolecules perform all of the active functions that we associate with life, from muscle contraction to sensing light and sound. Like the machines we are used to operating on macroscopic scales, these molecular machines have many moving parts that are essential to their function and dysfunction. This course introduces a framework for reasoning about such dynamics and computational tools for interrogating them.	
Topics Covered	The course introduces the concept of energy landscapes. Then it focuses on physics-based methods for simulating dynamics on such landscapes and analysis methods for extracting insight into biomolecular dynamics from such simulations.	
Course Objectives	The goal of this course is to prepare students for research using computational tools to understand biomolecular dynamics.	
Relationships of course objectives to Program Educational Objectives (Undergrad courses only)		
Contribution towards Student Outcomes (Undergrad courses only)	Check all that apply below/List here	
Weekly/Session Schedule	Week 1 Energy landscapes Week 2 Simulation methods Week 3 Enhanced sampling Week 4 Dimensionality reduction Week 5 Allostery and information theory Week 6 Markov state models (MSMs) Week 7 Comparing to experiments Week 8 Learning from simulations Week 9 Structure prediction Week 10 Drug design Week 11 Protein design Week 12 Hands-on project Week 13 Hands-on project Week 14 Hands-on project	

Grading details - types of assessments and weights	Participation in discussion 50% Project 50%
Prepared By/Date	Gregory R. Bowman 8/29/23

Student Outcomes

☐ **N/A**

☐ **1. An ability to identify, formulate, and solve complex engineering problems by applying principles of engineering, science, and mathematics.**

☐ **2. An ability to apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factors.**

☐ **3. An ability to communicate effectively with a range of audiences.**

☐ **4. An ability to recognize ethical and professional responsibilities in engineering situations and make informed judgments, which must consider the impact of engineering solutions in global, economic, environmental, and societal contexts.**

☐ **5. An ability to function effectively on a team whose members together provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives.**

☐ **6. An ability to develop and conduct appropriate experimentation, analyze and interpret data, and use engineering judgment to draw conclusions.**

☐ **7. An ability to acquire and apply new knowledge as needed, using appropriate learning strategies.**