

**Course Approval Form** 

For approval of new courses and deletions or modifications to an existing course.

registrar.gmu.edu/facultystaff/curriculum

Action Requested: X Create new course Delete ex Modify existing course (check all that apply Title Credits Prereq/coreq Schedule Type Other:	isting course ) Repeat Status Restrictions	Grade Type	Course Level: Undergraduate X Graduate	
College/School:       College of Science         Submitted by:       Dmitri Klimov		Department: School c Ext: 3-8395	f Systems Biology Email: dklimov@gmu.edu	
Subject Code: BINF Number: (Do not list multiple codes or numbers. Each course pro have a separate form.)	641 posal must	Effective Term: Fall X Spring Summ		
Title: Current Biomolecular Modeling Banner (30 characters max including spa New	ces) Biomole	ecular Modeling		
Credits:3Fixedor(check one)Variableto	Repeat Status: (check one)	X Not Repeatable (NR) Repeatable within degree Repeatable within term (		
Grade Mode: X Regular (A, B, C, etc.) (check one) Satisfactory/No Credit Special (A, B C, etc. +IP)	Schedule Type Code( (check all that apply)	s): Lecture (LEC) Lab (LAB) Recitation (RCT) Internship (INT)	Independent Study (IND) Seminar (SEM) Studio (STU)	
			Instructional Mode:	
Prerequisite(s): Students are expected to be familiar with basic concepts of physics, calculus, and biology on undergraduate level. Access to PC with internet connection is required.	Corequisite(s):		100% face-to-faceHybrid: ≤ 50% electronicallyx100% electronically delivered	
Special Instructions: (list restrictions for majo	pr/college/degree/prer	eg to be enforced by Banner)	Are there equivalent cours	e(s)?
none		• • •	Yes X No	. ,
			If yes, please list	
Cotolog Conv for NEW Courses	<b>Delve</b> (Conquit Linius	visity Catalog for models)		
Catalog Copy for NEW Courses ( Description (No more than 60 words, use verb p			information for the course)	
Introduction to basic principles and practice of co modeling. Students learn the elements of physica biology, which constitute the foundation of molecu application of biomolecular software and develop emphasized through online lectures, homework, a	mputational biomolecu I chemistry and molecu ular modeling. Practica ment of related skills a and course project.	ular cular al are		
	Hours of Lecture or Se all x Summer	eminar per week: 3	Hours of Lab or Studio:	
Approval Signatures				
Department Approval	Date	College/School Approval	Date	
If this course includes subject matter currentl those units and obtain the necessary signatures p				review by
	roval Name	Unit Approver's Signatu		
For Graduate Courses Only				
Graduate Council Member Provost Office			Graduate Council Approval Date	

For Registrar Office's Use Only: Banner\_

\_Catalog\_

revised 11/8/11

# Course Proposal Submitted to the Curriculum Committee of the College of Science

## 1. COURSE NUMBER AND TITLE: BINF641 Biomolecular modeling

<u>Course Prerequisites</u>: Students must be familiar with the basic concepts of physics, calculus, and biology on undergraduate level. Access to PC with internet connection is required.

<u>Catalog Description</u>: Introduction to basic principles and practice of computational biomolecular modeling. Students will learn the elements of physical chemistry and molecular biology, which together constitute the foundation of molecular modeling. Practical application of biomolecular software and development of related skills are emphasized through lectures, homework, and course project. The course is delivered entirely online via recorded lectures and meetings.

## 2. <u>COURSE JUSTIFICATION</u>:

<u>Course Objectives</u>: This course is designed for the students with the background in biology, chemistry, or computer science and who are interested in learning biomolecular modeling. The goal of the course is to introduce the principles of biomolecular modeling and develop practical skills using existing modeling software.

<u>Course Necessity</u>: Biomolecular modeling is a standard tool used in modern molecular biology, which allows one to address diverse problems from protein and RNA folding to biomolecular interactions in cellular environment and membrane transport. This approach is unique in its ability to provide detailed atomistic description of biomolecular systems, which complements experiments. The course will train students in this novel field and develop necessary practical skills. It is expected that completion of this course will improve employment prospects of the students on the job market.

<u>Course Relationship to Existing Programs</u>: This course will be included in the online versions of Bioinformatics and Computational Biology Graduate Certificate and MS in Bioinformatics and Computational Biology. These online programs are currently being developed.

<u>Course Relationship to Existing Courses</u>: At the present time GMU does not offer similar courses. The proposed course has partial (about 30%) overlap with existing graduate course BINF740 Introduction to Biophysics. However, the proposed course is entirely focused on the principles of biomolecular modeling with the emphasis on developing practical skills in software application. In contrast, BINF740 does not address practical use of software and it covers all fields of biophysics well beyond biomolecular aspects. The level of presentation in BINF740 is more advanced, because this course is required for PhD Program in Bioinformatics and Computational Biology. In addition, the curriculum of BINF641 is specifically designed for online asynchronous delivery, whereas BINF740 is a "traditional" classroom course.

### 3. APPROVAL HISTORY: none

## 4. <u>SCHEDULING AND PROPOSED INSTRUCTORS</u>:

## Semester of Initial Offering: Spring 2014

**Proposed Instructors:** Dmitri Klimov

# 5. <u>TENTATIVE SYLLABUS</u>: See attached

Syllabus for the proposed new online course BINF641

# BINF641: Biomolecular Modeling Instructor: Dmitri Klimov

**Course objective:** This course is designed for the students with the background in biology, chemistry, or computer science and who are interested in learning biomolecular modeling. The goal of the course is to introduce the principles of biomolecular modeling and develop practical skills using existing modeling software.

<u>Course description</u>: The course consists of two parts. The first part starts with the introduction of fundamental concepts of physical chemistry, which are commonly used in the description of biological systems. Molecular interactions, from covalent bonding to electrostatic and van-der-Waals interactions, are discussed. The course shows how these interactions are combined to produce a complex array of biomolecular structures found in DNA, RNA, proteins, and lipid cellular membranes. The molecular mechanisms of protein folding are discussed in detail. The unfolding of proteins implicated in a variety of biological functions is also introduced. The consequences of protein aggregation are explored and linked to a new class of diseases. Cellular defensive mechanisms against protein misfolding and aggregation, including chaperone systems, are presented.

The second part of the course describes the basic principles in biomolecular modeling, such as molecular mechanics. Practical implementation of biomolecular modeling, including the application of relevant simulation and visualization software, is emphasized. Several case studies illustrating the use of biomolecular modeling are discussed, including ligand binding and protein interactions with cellular membranes. As a final exam the students complete the course project on biomolecular modeling.

*Prerequisites*: Students are expected to be familiar with basic concepts of physics, calculus, and biology on undergraduate level. Access to PC with internet connection is required.

Grading basis: Students will be graded on the basis of homework (50%) and final exam (50%).

### Course materials:

- 1. Rodney Cotterill "Biophysics: An introduction"
- 2. Online lecture notes

Instructor: Dmitri Klimov Occoquan Building, Room 328C, Prince William Campus 703-993-8395 dklimov@gmu.edu Office hours: 2-3pm Monday or by appointment

<u>Academic Honesty Policy</u>: Students are expected to follow the Honor Code. Academic dishonesty will not be tolerated in this class. Exams, projects, and homework must reflect individual work. If you have difficulty with the assignments, discuss it with the instructor.

If you are a student with a disability and you need academic accommodations, please see me and contact the Office of Disability Resources at 703/993-2474. All academic accommodations must be arranged through that office.

#### Tentative course schedule:

#### Lecture 1

Elements of thermodynamics and statistical mechanics.

#### Lecture 2

Reaction kinetics and transport processes. Connecting thermodynamics and kinetics.

#### Lecture 3

Biomolecular interactions.

#### Lecture 4

Biomolecular structure: DNA, RNA, polypeptides.

#### Lecture 5

Biomolecular structure: Lipid membranes.

#### Lecture 6

Protein folding

#### Lecture 7

Mechanical unfolding of proteins as biological function

#### Lecture 8

Protein aggregation

#### Lecture 9

Preventing protein misfolding and aggregation

## Lecture 10

Proteins in cells: Molecular crowding

#### Lecture 11

Principles of biomolecular modeling

#### Lecture 12

Biomolecular modeling in practice: Using software applications

#### Lecture 13

Course project on biomolecular modeling

### Lecture 14

Biomolecular modeling as a research tool: (i) ligand binding to proteins, (ii) protein interactions with cellular membranes