George Mason University  
Graduate Course Approval/Inventory Form

Please complete this form and attach a copy of the syllabus for new courses. Forward it as an email attachment to the Secretary of the Graduate Council. A printed copy of the form with signatures should be brought to the Graduate Council Meeting. Complete the Coordinator Form on page 2, if changes in this course will affect other units.

Please indicate:  ___X___ NEW  ___ MODIFY  ___ DELETE

Local Unit:  SCS  
Graduate Council Approval Date:

Course Designation:  BINF  
Course Number:  841

Full Course Title:  Research Topics in Biomolecular Simulations

Abbreviated Course Title (24 characters max.):  Biomolecular Simulations

Credit hours:  3  
Program of Record:  Bioinformatics Ph.D.

Repeatable for Credit?  
___ D=Yes, not within same term  Up to hours  
___ T=Yes, within the same term  Up to  hours  
___ N=N=Cannot be repeated for credit

Activity Code:  ___X___ Lecture (LEC)  ___ Lab (LAB)  ___ Recitation (RCT)  
___ Studio (STU)  ___ Internship (INT)  ___ Independent Study (IND)  ___ Seminar (SEM)

Catalog Credit Format:  3:3:0  
Course Level:  GF(500-600) ___ GA(700+) ___

Maximum Enrollment:  10  
For NEW courses, first term to be offered:  Spring 2006

Prerequisites:  BINF 741 or Permission of Instructor

Catalog Description (35 words or less):  Research oriented course combining lectures and work on individual projects in biomolecular simulations. The topics include, but not limited to, protein and peptide aggregation, binding, unfolding and folding.

For MODIFIED or DELETED courses as appropriate:

Last term offered:  
Previous Course Abbreviation:  
Previous number:

APPROVAL SIGNATURES:

Submitted by:  
email: ________________

Department/Program:  
Date: ________________

College Committee:  
Date: ________________

Graduate Council Representative:  
Date: ________________
GEORGE MASON UNIVERSITY
Course Coordination Form

Approval from other units:

Please list those units outside of your own who may be affected by this new, modified, or deleted course. Each of these units must approve this change prior to its being submitted to the Graduate Council for approval.

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Graduate Council approval: _____________________________ Date: __________

Graduate Council representative: __________________________ Date: __________

Provost Office representative: __________________________ Date: __________
1. COURSE NUMBER AND TITLE:

BINF 841 – Research topics in Biomolecular Simulations

Prerequisites: BINF 741 or Permission of Instructor.

Catalog Description: Research oriented course combining lectures and work on individual projects in biomolecular simulations. The topics include, but not limited to, protein and peptide aggregation, binding, unfolding and folding.

2. COURSE JUSTIFICATION:

Course objectives: This course is designed for the students, who are interested in computer simulations of biomolecules. The goal is to introduce students to cutting-edge research work in computer simulations on the basis of individual research projects. Each of the projects represents a small novel problem, which offers the potential for new original results. To maximize the productive participation of students in their research, the course emphasizes individual work with the instructor. Suggested research topics include a wide range of problems in the area of protein structure dynamics, folding and unfolding, docking, and aggregation. Students may also select several computational approaches, from molecular dynamics to Langevin dynamics or Monte Carlo simulations.

Course Necessity: There is no such course in SCS or in GMU addressing the advanced study of computer simulations of biomolecules on the graduate level. This exposes students to advanced topic in a very important area of bioinformatics and computational biology

Course Relationship to Exiting Programs: This course is currently offered (Spring 05) as BINF 739 Special Topics. It will be an elective course for students in the Ph.D. or the MS in Bioinformatics Programs

Course Relationship to Existing Courses: There is no similar course at GMU.

3. APPROVAL HISTORY: NA

4. SCHEDULING AND PROPOSED INSTRUCTORS:

Semester of Initial Offering: Spring 2006

Proposed instructors: Dr. Dmitri Klimov

5. TENTATIVE SYLLABUS: See attached.
BINF 841: Research Topics in Biomolecular Simulations
Instructor: Dmitri Klimov
Prince William Discovery Hall 185
1:30-4:10 pm Tues

Course Description: This course is designed for the students, who are interested in computer simulations of biomolecules. The goal is to introduce students to cutting-edge research work in computer simulations on the basis of individual research projects. Each of the projects represents a small novel problem, which offers the potential for new original results. To maximize the productive participation of students in their research, the course emphasizes individual work with the instructor. Suggested research topics include a wide range of problems in the area of protein structure dynamics, folding and unfolding, docking, and aggregation. Students may also select several computational approaches, from molecular dynamics to Langevin dynamics or Monte Carlo simulations.

The structure of the course is as follows. The course begins with the four introductory lectures, describing the background in suggested research topics as well computational methodologies and software. Students will select one of the topics or may propose their own topic. After the approval from the instructor they perform literature search and write a short research proposal, describing the current research and the objective of their project. The students work on their projects and upon completion write a report in the format of a scientific paper and make a presentation. During this course the instructor will provide guidance and assistance and intensive interaction between students and instructor is expected.

Prerequisites: Good knowledge of a computer programming language (Fortran, C, or Java) is required. It is also expected that students have a basic knowledge of protein structure and properties. Previous experience in molecular simulations is not assumed.

Grading basis: The course grade is based on literature research (25%), commitment and efforts in completing the research projects (50%), and final report and presentation (25%).

Suggested research projects:

1. Conformational properties of polypeptides implicated in amyloidogenic diseases (molecular dynamics)
2. Docking of polypeptides (molecular dynamics)
3. Temperature induced unfolding (molecular dynamics)
4. Force induced unfolding (molecular dynamics)
5. Peptide fibrillation (Monte Carlo)
6. Protein folding of nanotubes (Langevin dynamics)