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: 741  

Full Course Title: Introduction to Computer Simulations of Biomolecules  

Abbreviated Course Title (24 characters max.): Biomolecule Simulation  

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:  

___ 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: 15  

For NEW courses, first term to be offered: Fall 2005  

Prerequisites: Graduate standing and good programming skills, BINF 690 and 701, or Permission of Instructor.  

Catalog Description (35 words or less):  
Computational methods in biomolecular simulations, such as molecular dynamics and Monte Carlo algorithm, are introduced in detail. Special emphasis is given to practical applications. The most recent advances in biomolecular simulations are reviewed.  

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 741 – Cellular Introduction to Computer Simulations of Biomolecules

Prerequisites: Graduate standing and good programming skills, BINF 690 (Numerical Methods for Bioinformatics) and BINF 701 (Biochemical Systematics), or permission from instructor.

Catalog Description: Computational methods in biomolecular simulations, such as molecular dynamics and Monte Carlo algorithm, are introduced in detail. Special emphasis is given to practical applications. The most recent advances in biomolecular simulations are reviewed.

2. COURSE JUSTIFICATION:

Course objectives: This course is intended to serve as an introduction to computational methods for simulating biological macromolecules, such as proteins, DNAs, and RNAs. It is designed for the students who are interested in computational biology and whose background is in physics, chemistry, biology, computer science, or mathematics.

Course Necessity: There is no such course in SCS or in GMU addressing the computer simulations of biomolecules on the graduate level. This area lays the foundations for a very important area of bioinformatics and computational biology

Course Relationship to Exiting Programs: This course is currently offered (Fall 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: Fall 2005

Proposed instructors: Dr. Dmitri Klimov

5. TENTATIVE SYLLABUS: See attached.
BINF 741: Introduction to Computer Simulations of Biomolecules

**Description:** This course is intended to serve as an introduction to computational methods for simulating biological macromolecules, such as proteins, DNAs, and RNAs. It is designed for the students who are interested in computational biology and whose background is in physics, chemistry, biology, computer science, or mathematics.

The **first part** of the course provides an overview of various “hot topics” in computational biology, in which computer simulations play an instrumental role. A minitutorial of the molecular structure of proteins, DNAs, and RNAs is also included. The basic principles of computational modeling of biomolecules are then discussed, including the construction of potential function (“force field”).

The **second part** examines Monte Carlo (MC) method, including the concept of importance sampling, detailed balance, Metropolis scheme, and selection of trial moves. Limitations and potential errors in implementing MC for biomolecules are discussed. The examples of MC programs used in biomolecular simulations are shown.

The **third part** introduces the idea of molecular dynamics (MD) method. Various algorithms for numerical solution of Newton equations of motion are evaluated. Special attention is given to numerical implementation of different simulation ensembles and efficient algorithms for computing long-range interactions. Practical application of MD simulations is demonstrated using NAMD software package.

The **forth part** of the course includes special topics, such as techniques to save computer time, the methods of enhancing conformational sampling and the analysis of simulation data (such as multiple histogram technique, measures of ergodicity of simulations, etc).

**Grading basis:** One of the main goals of the course is to provide practical experience with MC and MD simulations. Instead of formal exams, students complete two simulation projects. The first project is focused on MC simulations of lattice protein model. The second project involves running “real life” MD simulations to characterize structural properties of short peptide sequences.

**Prerequisites:** Students are expected to be familiar, on an undergraduate level, with basic concepts in physics, calculus, and programming language suitable for numerical computations (such as Fortran or C). Knowledge of biological aspects of simulations is not required.