BINF690: *Numerical Methods in Bioinformatics*

Course Time: Mondays, 4:30 pm - 7:10 pm

Location: Innovation Hall, Room 333, Fairfax Campus

Instructor: Dmitri Klimov
Occoquan Building, Room 328B, Prince William Campus
703-993-8395
dklimov@gmu.edu
Office hours: by appointment

Required textbook: *Numerical Methods for Engineers* by Chapra and Canale (5th or 6th editions)

Class website: www.binf.gmu.edu/dklimov

Course Description: The course introduces the foundations of computational techniques for solving scientific problems. The practical implementation of numerical techniques for "real-life" problems in computational biology is demonstrated. Students will develop the ability to convert a quantitative problem into computer programs.

Prerequisites: Elementary calculus and knowledge of a programming language. An understanding of the basic concepts of linear algebra and introductory differential equations is helpful.

Grading Policy:
Homework 40%
Midterm classroom exam (open book policy) 30%
Final take-home exam or project 30%

Late assignments will not be accepted unless due to emergency or work-related reason (for working students).

Academic Honesty Policy: 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.

Course schedule for Fall 2013

Lecture 1, Aug 26
Numerical methods in science. Programming and implementation of numerical methods (Chapters 1-3).

Lecture 2, Sep 9
Taylor series. Error propagation (Chapter 4).

Lecture 3, Sep 16
Roots of equations (Chapters 5 and 6).

Lecture 4, Sep 23
Linear algebraic equations (Chapter 9)

Lecture 5, Sep 30
Optimization and minimization (Chapters 13 and 14)

Lecture 6, Oct 7
Curve fitting (Chapters 17 and 18)

Lecture 7, Oct 15
Midterm classroom exams

Lecture 8, Oct 21
Numerical differentiation and integration (Chapters 21 and 23)

Lecture 9, Oct 28
Solution of ordinary differential equations (Chapter 25)

Lecture 10, Nov 4
Boundary-value and eigenvalue problems (Chapter 27)

Lecture 11, Nov 11
Numerical methods: Molecular dynamics (online lecture notes)

Lecture 12, Nov 18
Numerical methods: Monte Carlo algorithm (online lecture notes)

Lecture 13, Nov 25
Application: Computation of energy for complex molecular systems (online lecture notes)
Application: Multistepping technique in solving differential equations (online lecture notes)

Lecture 14, Dec 2
Advanced numerical techniques (online lecture notes)

Final exams will be held during exam week.

Notes:

1. Each lecture is a 2 ½ hour presentation with a 10 minutes break.
2. The chapters refer to the class textbook *Numerical Methods for Engineers* by Chapra and Canale.