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

Location: Ball Run Hall, Room 248, Prince William Campus

Instructor: Dmitri Klimov
Occoquan Building, Room 328C
703-993-8395
dklimov@gmu.edu
Office hours: 3-4pm Monday or by appointment

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

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 2009

Lecture 1, Aug 31
Numerical methods in science. Programming and implementation of numerical methods (Chapters 1-3).

Lecture 2, Sep 14
Taylor series. Error propagation (Chapter 4).

Lecture 3, Sep 21
Roots of equations (Chapters 5 and 6).

Lecture 4, Sep 28
Linear algebraic equations (Chapter 9)

Lecture 5, Oct 5
Optimization and minimization (Chapters 13 and 14)

Lecture 6, Oct 13
Midterm exams

Lecture 7, Oct 19
Curve fitting (Chapters 17 and 18)

Lecture 8, Oct 26
Numerical differentiation and integration (Chapters 21 and 23)

Lecture 9, Nov 2
Solution of ordinary differential equations (Chapter 25)

Lecture 10, Nov 9
Boundary-value and eigenvalue problems (Chapter 27)

Lecture 11, Nov 16
Numerical methods: Molecular dynamics (online lecture notes)

Lecture 12, Nov 23
Numerical methods: Monte Carlo algorithm (online lecture notes)

Lecture 13, Nov 30
Application: Computation of energy for complex molecular systems (online lecture notes)
Application: Multisteping technique in solving differential equations (online lecture notes)

Lecture 14, Dec 7
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.