BINF 690 Numerical Methods in Bioinformatics

Course syllabus

Course Time: Mondays, 4:30 pm - 7:10 pm
Location: Bull Run Hall, Room 252, Prince William Campus
Instructor: Dmitri Klimov
Occoquan Building, Room 328C
703-993-8395
dklimov@gmu.edu

Textbook: *Numerical Methods for Engineers* by Chapra and Canale (Fifth edition)

Class website: www.iiinf.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 Exam 30%
Final Exam 30%

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.

http://www.argitect.com/folding/nummethods/nummethods_show.htm?doc_id=510748
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Course schedule Fall 2008

http://www.orchestration.com/fool/mg/nunmethods/munmethrods_show.htm?id=510749
Lecture 1, Aug 25
Numerical methods in science. Programming and implementation of numerical methods (Chapters 1-3).

Lecture 2, Sep 8
Taylor series. Error propagation (Chapter 4).

Lecture 3, Sep 15
Roots of equations (Chapters 5 and 6).

Lecture 4, Sep 22
Linear algebraic equations (Chapter 9)

Lecture 5, Sep 29
Optimization and minimization (Chapters 13 and 14)

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

Lecture 7, Oct 14
Midterm exams

Lecture 8, Oct 20
Numerical differentiation and integration (Chapters 21 and 23)

Lecture 9, Oct 27
Solution of ordinary differential equations (Chapter 25)

Lecture 10, Nov 3
Boundary-value and eigenvalue problems (Chapter 27)

Lecture 11, Nov 10
Numerical methods: Molecular dynamics (online lecture notes)

Lecture 12, Nov 17
Numerical methods: Monte Carlo algorithm (online lecture notes)

Lecture 13, Nov 24
Application: Computation of energy for complex molecular systems (online lecture notes)
Application: Multisteping technique in solving differential equations (online lecture notes)

Lecture 14, Dec 1
Advanced numerical techniques (online lecture notes)

Final exams will be held during exam week.
Notes:

1. Each lecture is a 2½ hour presentation with a 10 minutes break.

2. The chapters refer to the class textbook Numerical Methods for Engineers by Chapra and Canale.