

Syllabus for BINF690: *Numerical Methods in Bioinformatics*

Name of course: BINF690 Numerical Methods in Bioinformatics

Meeting place: Bull Run Hall, Room 252, S&T Campus

Meeting time: Mondays, 4:30 pm - 7:10 pm

Instructor Name: Dmitri Klimov

Credits: 3

Class website: <http://binf.gmu.edu/dklimov/nummethods.html> and on Blackboard
(201770 - Master - BINF-690-003 / BINF-690-DL3 / CSI-690-003)

Office location: Colgan Hall, Rm 328B, Science and Technology Campus (PWC)

Office hours: By appointment (email to set up an in-person appointment or to speak over the telephone)

Email address: dklimov@gmu.edu (preferred way of communication)

Telephone number: 703-993-8395

Course Description and Goals

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 emphasized. Students will develop an ability to convert a quantitative problem into computer programs.

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

Required Reading

Required textbook: *Numerical Methods for Engineers* by Chapra and Canale, preferably, 5th, 6th or 7th editions. If using other editions, please contact the instructor.

Course Policies

Grading scale (points): A+ (>100), A (90-100), B (80-89), C (\leq 79)

Grading policy: Students will be graded on the basis of homework (30%), midterm classroom exam (open book policy) (25%), final take-home exam or project (25%), and class participation (20%). For each problem or assignment a student will earn up to one point.

Late assignments: Late assignments will not be accepted unless due to emergency, work-related or other documented reasons.

Other considerations: If there are any schedule issues related to religious holidays, please inform the instructor the first week of class. Completion of regular weekly homework is expected to take several hours.

Learning Outcomes

By the end of this course, students will be able to

1. apply various algorithms for solving numerical problems in computational biology
2. appraise theoretical foundations of algorithms
3. develop practical skills for writing computer programs solving numerical problems
4. perform elementary molecular simulations

Course Logistics

The course uses Blackboard for distributing lecture materials, submission of homework, grading, and, for distance learning students, for accessing online sessions.

To Access Blackboard

1. Go to <http://mymason.gmu.edu>.
2. Login using your NETID and password.
3. Click on the ‘Courses’ tab.
4. Click on “201770 - Master - BINF-690-003 / BINF-690-DL3 / CSI-690-003 (Fall 2017)” under the “Course List” heading.

Technology Requirements for the Course

Hardware: You will need access to a Windows, Macintosh or Linux computer with at least 2 GB of RAM and to a fast and reliable broadband internet connection (e.g., cable, DSL). A larger screen is recommended for better visibility of course material. Students will need speakers or headphones to hear recorded content and a headset with a microphone is highly recommended for best experience.

Software: This course uses Blackboard as a learning management system. You will need a browser and operating system that are listed compatible or certified with the Blackboard version available on the myMason Portal. Log in to myMason to access BINF690. You may need Acrobat Reader, Flash, Java (Windows), and Windows Media Player, QuickTime and/or Real Media Player. Your computer should be capable of running current versions of those applications. Also, make sure your computer is protected from viruses by downloading the latest version of Symantec Endpoint Protection/Anti-Virus software for free at <http://antivirus.gmu.edu/>.

Students owning Macs or Linux should be aware that some courses may use software that only runs on Windows. You can set up a Mac computer with Boot Camp or virtualization software so Windows will also run on it. Computers running Linux can also be configured with virtualization software or configured to dual boot with Windows.

Note: If you are using an employer-provided computer or corporate office for class attendance, please verify with your systems administrators that you will be able to install the necessary applications and that system or corporate firewalls do not block access to any sites or media types.

Course-specific Hardware/Software: Students are expected to have access to any programming language suitable for scientific calculations (C, Fortran, Java, perl etc).

Technical Help: If you have difficulty with accessing Blackboard, please contact the ITS Support Center at 703.993.8870 or support@gmu.edu. If you have trouble with using the features in Blackboard, email courses@gmu.edu.

Student Responsibilities

MasonLive/Email: Students are responsible for the content of university communications sent to their George Mason University email account and are required to activate their account and check it regularly. All communication from the university, college, school, and program will be sent to students solely through their Mason email account.

Students with disabilities: Students with disabilities who seek accommodations in a course must be registered with the George Mason University Disability Services and inform their instructor, in writing, at the beginning of the semester [See Disability Services website: <http://ds.gmu.edu/>].

Academic integrity: Students must be responsible for their own work, and students and faculty must take on the responsibility of dealing explicitly with violations. The tenet must be a foundation of our university culture [See Academic Integrity website: <http://oai.gmu.edu/>].

Honor Code and Virtual Classroom Conduct: Students must adhere to the guidelines of the George Mason University Honor Code [See Honor Code website: <http://oai.gmu.edu/mason-honor-code/full-honor-code-document/>].

Academic Honesty Policy of the course: 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.

University policies: Students must follow the university policies [See University Policies website: <http://universitypolicy.gmu.edu>].

Responsible use of computing: Students must follow the university policy for Responsible Use of Computing [See University Policies website: <http://universitypolicy.gmu.edu/policies/responsible-use-of-computing>].

University calendar: Students should consult the current Academic Calendar [See University Calendar website: <https://www2.gmu.edu/academics/academic-calendar>].

University catalog: Students should use the current university catalog [See University Catalog website: <http://catalog.gmu.edu>].

Student Services

Writing center: The George Mason University Writing Center staff provides a variety of resources and services (e.g., tutoring, workshops, writing guides, handbooks) intended to support students as they work to construct and share knowledge through writing. (See Writing Center website: <http://writingcenter.gmu.edu>). ESL Help: The program was designed specifically for students whose first language is not English who feel they might benefit from additional, targeted support over the course of an entire semester.

University libraries: University Libraries provide resources for distance learning students [See Library website: <http://library.gmu.edu/distance>].

Counseling and Psychological Services: The George Mason University Counseling and Psychological Services (CAPS) staff consists of professional counseling and clinical psychologists, social workers, and counselors who offer a wide range of services (e.g., individual and group counseling, workshops and outreach programs) to enhance students' personal experience and academic performance [See Counseling and Psychological Services website: <http://caps.gmu.edu>].

Family Educational Rights and Privacy Act (FERPA): The Family Educational Rights and Privacy Act of 1974 (FERPA), also known as the "Buckley Amendment," is a federal law that gives protection to student educational records and provides students with certain rights [See Registrar's Office website: <http://registrar.gmu.edu/privacy>].

Course schedule for Fall 2017

Lecture 1, Aug 28

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

Lecture 2, Sep 11

Taylor series. Error propagation (Chapter 4).

Lecture 3, Sep 18

Roots of equations (Chapters 5 and 6).

Lecture 4, Sep 25

Linear algebraic equations (Chapter 9)

Lecture 5, Oct 2

Optimization and minimization (Chapters 13 and 14)

Lecture 6, Oct 10

Midterm classroom exam

Lecture 7, Oct 16

Curve fitting (Chapters 17 and 18)

Lecture 8, Oct 23

Numerical differentiation and integration (Chapters 21 and 22)

Lecture 9, Oct 30

Solution of ordinary differential equations (Chapter 25)

Lecture 10, Nov 6

Boundary-value and eigenvalue problems (Chapter 27)

Lecture 11, Nov 13

Numerical methods: Molecular dynamics (online lecture notes)

Lecture 12, Nov 20

Numerical methods: Monte Carlo algorithm (online lecture notes)

Lecture 13, Nov 27

Application: Computation of energy for complex molecular systems (online lecture notes)

Application: Multisteping technique in solving differential equations (online lecture notes)

Lecture 14, Dec 4

Advanced numerical techniques (online lecture notes)

Notes:

1. Each lecture is a 2 ½ hour presentation with a 10-minute break.

2. The chapters refer to the class textbook *Numerical Methods for Engineers* by Chapra and Canale.
3. Final exam will be held during exam week.