Syllabus for BINF690: *Numerical Methods in Bioinformatics*

Name of course: BINF690 Numerical Methods in Bioinformatics
Meeting place: online
Meeting time: Mondays, 4:30 pm - 7:10 pm
Instructor Name: Dmitri Klimov
Credits: 3
Class website: Blackboard 202370.72179 BINF-690-DL1 (Fall 2023)
Office location: Colgan Hall, Rm 328B, Science and Technology Campus (PWC)
Office hours: By appointment (email to arrange virtual zoom meeting 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: 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, 5 through 8th editions.

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 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. Homeworks are weighted equally independent of the number of problems.

Campus Closure: If the campus closes or class is canceled due to weather or other concern, students should check Blackboard and/or contact instructor for updates on how to continue learning and information about any changes to events or assignments.

Participation and make-up work: In case of illness or quarantine, please contact the instructor to set up a plan for make-up work. Late assignments will not be accepted unless due to emergency, illness, quarantine, work-related or other documented reasons.

Course Recordings: All synchronous meetings in this class will be recorded to provide necessary information for students in this class. Recordings will be stored on Blackboard and will only be accessible to students taking this course during this semester.

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 to 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 basic computer 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 https://mymasonportal.gmu.edu.
2. Login using your NETID and password.
3. Click on the 'Courses" tab.
4. Click on "**202370.72179 BINF-690-DL1 (Fall 2023)"** in the Course List.

Technology Requirements for the Course

Software and Hardware: This course uses Blackboard as a learning management system available at https://mymasonportal.gmu.edu. Students are required to have regular, reliable access to a computer with an updated operating system (recommended: Windows 10 or 11 or Mac OSX 10.13 or higher) and a stable broadband Internet connection (cable modem, DSL, satellite broadband, etc., with a consistent 1.5 Mbps [megabits per second] download speed or higher). Activities and assignments in this course will regularly use web-conferencing software (Blackboard Collaborate Ultra). In addition to the requirements above, students are required to have a device with a functional camera and microphone. A larger screen is recommended for better visibility of course material. In an emergency, students can connect through a telephone call, but video connection is the expected norm.

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, perl, python 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

Mason 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: https://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: https://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: https://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 Policy website: https://universitypolicy.gmu.edu].

Responsible use of computing: Students must follow the university policy for Responsible Use of Computing [See University Policy website: https://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: https://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: https://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/for/online].

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: https://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: https://registrar.gmu.edu/ferpa/].

Course Materials and Student Privacy

Video recordings of class meetings that are shared only with the instructors and students officially enrolled in a class do not violate FERPA or any other privacy expectation. Video recordings that only include the instructor (no student names, images, voices, or identifiable texts) may be shared without violating FERPA (but see University Policies: Privacy, for some qualifications and recommendations). All course materials posted to Blackboard or other course site are private to this class; by federal law, any materials that identify specific students (via their name, voice, or image) must not be shared with anyone not enrolled in this class.

Video conferencing or recordings: Video recordings - whether made by instructors or students - of class meetings that include audio, visual, or textual information from other students are private and must not be shared outside the class. Live video conference meetings (e.g., Collaborate Ultra) that include audio, textual, or visual information from

other students must be viewed privately and not shared with others in your household or recorded and shared outside the class.

Course schedule for Fall 2023

Lecture 1, Aug 21
Numerical methods in science. Programming and implementation of numerical methods (Chapters 1-3).

Lecture 2, Aug 28
Taylor series. Error propagation (Chapter 4).

Lecture 3, Sep 11
Roots of equations (Chapters 5 and 6).

Lecture 4, Sep 18
Linear algebraic equations (Chapter 9)

Lecture 5, Sep 25
Optimization and minimization (Chapters 13 and 14)

Lecture 6, Oct 2
Curve fitting (Chapters 17 and 18)

Lecture 7, Oct 10
Midterm classroom exam

Lecture 8, Oct 16
Numerical differentiation and integration (Chapters 21 and 22)

Lecture 9, Oct 23
Solution of ordinary differential equations (Chapter 25)

Lecture 10, Oct 30
Boundary-value and eigenvalue problems (Chapter 27)

Lecture 11, Nov 6
Numerical methods: Molecular dynamics (online lecture notes)

Lecture 12, Nov 13
Numerical methods: Monte Carlo algorithm (online lecture notes)

Lecture 13, Nov 20
Application: Computation of energy for complex molecular systems (online lecture notes)
Application: Multistepping technique in solving differential equations (online lecture notes)

Lecture 14, Nov 27
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.