CSI 780 *Principles of Modeling and Simulation in Science*
Fall 2021

Modality: Synchronous online Zoom video-conference
Class time: Tuesdays, 4:30 pm - 7:10 pm

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Office location: Research Hall 221, Fairfax campus
Office hours: By appointment, all meetings through Zoom
Email address: blaisten@gmu.edu (preferred way of communication)

- ***The class modality is synchronous/online.*** *Activities and assignments in this course will regularly use web-conferencing software (Zoom). Students are required to have a laptop/desktop with a functional camera and microphone. In an emergency, students can connect through a telephone call, but video connection is the expected norm.*

- *Students are required to follow Mason's current policy about facemask-wearing. As of August 11, 2021,* ***all community members are required to wear a facemask in all indoor settings, including classrooms****. An appropriate facemask must cover your nose and mouth at all times in our classroom. If this policy changes, you will be informed; however, students who prefer to wear masks consistently will always be welcome for any departmental activity that entails inside gatherings.*
- *If the* ***campus closes****, or if a* ***class meeting needs to be canceled*** *or adjusted due to weather or other concern,* ***students should check the course website and your email for updates*** *on how to continue learning and for information about any changes to events or assignments.*
- ***Professor Blaisten does not authorize in anyway the recording*** *of any lecture content in this course. Sharing of video lecture or lab content violates student privacy governed by the Family Education Rights and Privacy Act (FERPA). Additionally, any written, video, or audio content built by Prof. Blaisten for CSI 780 instruction that is shared online externally to GMU is a clear and punishable violation of GMU's Honor Code.*

Course Description and Goals

The theme of the course is a set of analytical methods that are routinely used in Modeling and Simulation in Science. These methods are currently orthodox means for modeling and simulating molecular-scale models of matter. The methods were originally implemented for computer applications in the 1950's, began to receive widespread attention in the mid-1970's, and are today a fundamental scientific approach to design nano systems, as well as bulk crystals, glasses, liquids, polymers, surfaces, and interfaces. Additionally, much of these methodologies have been adopted by computational biologists, and are today an essential element of bio-oriented research.

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

1. apply numerical algorithms for solving numerical problems that arise in computational science
2. appraise theoretical foundations of algorithms

3. reinforce practical skills for building computer programs that include common data analysis of the simulation methods learned in class
4. perform elementary simulations

Prerequisites: Calculus, introductory physics or physical chemistry, and knowledge of a programming language (at the level of CSI 501 or better). An understanding of the basic concepts of ordinary differential equations is helpful.

Required Textbook

- ***A first course in Computational Physics***, 2nd edition, by Paul DeVries and Javier Hasbun, Jones & Bartlett (1st edition can be found online)

Supplementary textbook, not required but recommended:

- ***Computational Physics***, 2nd edition, by Nicholas Giordano and Hisao Nakanishi, Prentice Hall (can be found online)

Extra references for "tools to coding"

Numerical Recipes by W. H. Press, B. P. Flannery, et al. Cambridge Press

FORTRAN 90 by Cooper Redwine, Springer.

Evaluation

Grading scale (points): A (90-100), B (80-89), C (≤79) (with eventual slight variations)

Grading policy (may change slightly):
1) 35% of the final grade from the work acquired through the homework on the textbook exercises and other provided exercises.
2) 35% of the final grade from the class projects left during the lectures as homework.
3) 30% of final grade acquired by class participation and attendance, including presentations by students on the material related to the textbook or class notes, on their advances in the projects, or additional explanations on homework assignments. Includes also a final presentation of the project as part of a presenter-team to take place on the date of final exam

- There will not be partial and final exams.

- Mason holds its students to a high degree of trust. The Honor Code is enforced in all activities.

- All cell phones should be turned off before the class starts and during the class time.

Late assignments: Late assignments will not be accepted unless due to emergency or work-related compelling reasons for part-time students.

"Re-do" homework policy:

1) Homework graded and returned to you can be revised for a better grade with a penalty on its final grade of minus 1 point.

2) Redo homework should be turned in with the original handout containing the corrections.

Other considerations: If there are any obligations related to religious holidays, please inform

the instructor the first week of class

Course schedule for Fall 2021

This is a hands-on course where there will be as little lecturing as possible.

The lectures will supplement textbook material by introducing a variety of the science concepts involved in various modeling and simulation areas where numerical methods are fundamental for computer modeling and simulation. A tentative list of subjects follows:

1) Models' classification
    -- Modeling processes
    -- Steps of the modeling process
2) Data driven models
    --Data interpolation
    --Curve fitting
    --Root finder algorithms
3) Computational error
    --Data modeling, implementation vs algorithmic errors, truncation errors
    --Error propagation, precision
    --Linear and non-linear fitting algorithms
4) Simulation techniques
    -_Simulating with randomness
    --Random number generators
    --Random walks
    --Monte Carlo integration
    --Sampling techniques: important sampling
    --Cellular automaton simulations
    --Case studies of percolation and aggregation mechanisms
5) Optimization as a simulation component
    --Genetic algorithms
    --Steepest descent algorithms
    --Applications to nanostructures
6) Dynamical simulation tools of the trade
    --Numerical solution of ordinary differential equations
    --Predictor-corrector techniques
    --Diffusing motion
    --Case study: chaotic behavior
    --Qualitative measures of chaos
7) Modeling continuum systems with partial differential equations
    --Heat equations, fluid flow equations, Hook's and Fourier's laws
    --Matrices and systems of algebraic equations for numerical solution of partial differential equations
8) Fourier analysis tools and applications
    --Time series: regular and irregular behavior
    --Spatial reconstruction, tomography, scattering
9) Case studies:
    i) Geometrical optimization of Morse clusters by steepest descent method

ii) Genetic algorithm optimization of Lennard Jones clusters
iii) Cellular automata: Eden cluster, epidemics growth, LDA aggregation
iv) Regular-to-Irregular transition: dynamical behavior as a function of a Hamiltonian parameter

10) Final presentations: Project presentations. Three student groups will be assigned to prepare and present one of the class projects in a final meeting date. This meeting is not an exam, it is part of the projects-homework and your contribution to class participation.

Homework and projects

The textbook chapter materials will be mostly worked out independently by each student. Along the semester, Students will be assigned to prepare individually short sections of either textbook, present those in class, and do the exercises contained therein.
A report per homework showing the achievements accomplished by every student will be required weekly, to be turned in in electronic format by email.

Every project report (and homework!) should be structured according to the following suggested scheme:
1) Title
2) Abstract
3) Introduction to the subject, stating the exercises that are solved in the rest of the report.
4) Model and methods used
5) Results of exercises and any extra finding of your own.
6) Conclusions and Observations
7) Bibliography
Three projects will be assigned as homework from material discussed in the lectures. A report will be due for each project. Towards the end of November, teams of students will be formed. Each team will be assigned to review thoroughly one of the projects already done, incorporate material from the textbook, present a consolidated report with the approaches of all team members, and prepare an oral presentation much in the way done in a scientific symposium.

Course Logistics

The course uses a password-protected site for distributing lecture materials and announcements. You will need to access the site remotely with a browser (Firefox, Safari, etc).

- **ID/password instructions will be sent by email to your GMU email.**

IT Requirements for the Course

Hardware: You will need access to a Windows, Macintosh, or Linux computer. The lab in RH 249 allows you to work in any of the 24 linux-servers, either in person or remotely through SSH (or Putty). You login with your Mason ID and password:

cdsXX.mesa.gmu.edu, where XX=01 through 24

These RH 249 computers do not share the desktops. Therefore, it is recommended that you take note on what computer you work the first time, and then keep working in that computer for the rest of the semester. To access these workstations remotely, you need to install the

Mason VPN (Virtual Private Network) and to be login to it. For the installation use:

https://its.gmu.edu/service/virtual-private-network-vpn/

Software: Computers in this lab have all the needed software. They have installed compilers for Fortran, C, c++. Python and MatLab. If computers in this lab are not used, students are expected to have access to a programming language software suitable for scientific calculations.

Course Policies: Student Responsibilities

Email: Students are responsible for reading and maintaining the content of university emails sent to their Mason email account. Therefore, students are required to maintain activate their email account and check it regularly. All communications from this course will be sent to students solely through their Mason email account.

Use of cell phones, cameras, recording, texting in class is not allowed. Students should turn off the ringing of smart devices (cell phone, alerts apps) while in either the in-person or Zoom classrooms.

- *The use of laptop or a desktop computer is required in this class. You will only be permitted to work on material related to the class, however. Engaging in activities not related to the course (e.g., gaming, email, chat, etc.) will result in a significant reduction in your participation grade.*
- *We will frequently be using computers for our "in-class" writing assignments. Please be respectful of your peers and your instructor and do not engage in activities that are unrelated to the class. Such disruptions show a lack of professionalism and may affect your participation grade.*

Academic integrity: Students are responsible for their own work and must take on the responsibility of dealing explicitly with consequences to any academic integrity violation. Students must adhere to the George Mason University **Honor Code** as it relates to integrity regarding coursework and grades. The Honor Code reads as follows:

"To promote a stronger sense of mutual responsibility, respect, trust, and fairness among all members of the George Mason University community and with the desire for greater academic and personal achievement, we, the student members of the University Community have set forth this: Student members of the George Mason University community pledge not to cheat, plagiarize, steal and/or lie in matters related to academic work."
[Honor Code website: https://oai.gmu.edu/mason-honor-code/full-honor-code-document/].

This is very important. [See Academic Integrity website: https://oai.gmu.edu/].

Classroom Conduct: Students must adhere to the Mason Honor Code and be very respectful of all class co-participants and instructor. It is recommended that remote students select a static virtual background for joining the classes. This enhances privacy. It is helpful for the group if each student adds a photo (ID type of photo) to be visible when the conference video is off.

Academic honesty policy of the course: Students are expected to follow the Honor Code at all time and for all activities. Academic dishonesty will not be tolerated in this class. Quizzes, questionnaires, projects, and homework must reflect individual work. If you have difficulty with the assignments, discuss them with the instructor.

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

Students that become ill: Students that become ill due to the pandemic should follow the Mason health recommendations and steps to follow: [https://shs.gmu.edu/.

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: https://universitypolicy.gmu.edu/policies/responsible-use-of-computing].

University calendar: Students should consult the current Academic Calendar. https://registrar.gmu.edu/calendars/fall_2021/

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

Student Services

University libraries: University Libraries provide excellent resources for books and journal publications. In addition, there are resources for distance students [See Library website, http://library.gmu.edu/for/online].

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.

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].