MATH*6020 Scientific Computing
Fall 2021
Section(s): C01s
Department of Mathematics & Statistics
Credit Weight: 0.50
Version 0.01 – September 1, 2021

Disclaimer

Please note that the ongoing COVID-19 pandemic may necessitate a revision of the format of course offerings, changes in classroom protocols, and academic schedules. Any such changes will be announced via CourseLink and/or class email.

This includes on-campus scheduling during the semester, mid-terms and final examination schedules. All University-wide decisions will be posted on the COVID-19 website (https://news.uoguelph.ca/2019-novel-coronavirus-information/) and circulated by email.

1 Course Details

1.1 Calendar Description

This course covers the fundamentals of algorithms and computer programming. This may include computer arithmetic, complexity, error analysis, linear and nonlinear equations, least squares, interpolation, numerical differentiation and integration, optimization, random number generators, Monte Carlo simulation; case studies will be undertaken using modern software.

1.2 Course Description

The course will be primarily concerned with the numerical solution of large sparse linear algebraic systems, both from a theoretical and an implementation point of view. Connections with optimisation problems, nonlinear systems of equations, numerical treatment of differential equations (e.g. via numerical differentiation and integration) will be discussed. The focus will be on iterative methods. Students will be expected to independently acquire the computational skills need for the programming assignments. A final course project will be carried out that requires the application of such techniques. A good preparation for this course will be familarity with solution theorey for linear algebraic systems and standard methods to solve them; prior exposure to numerical methods and their programming will also be of advantage but is not necessarily required.

1.3 Timetable

MON,WED – 13:00-14:20, via zoom (cf courselink)

This is a synchronous online course with lectures delivered via video conferencing. Login information will be provided to registered students through courselink.

Timetable is subject to change. Please see WebAdvisor for the latest information.

1.4 Final Exam

Oral examinations will be held, via zoom, tentatively on December 15, 2021 or on another mutually agreed upon (by instructor and student) day. A detailed exam schedule will be provided in the last one or two weeks of classes.

2 Instructional Support

Instructor: Hermann Eberl
Email: heberl@uoguelph.ca
Office Hours: WED 16:00-17:00 (by appointment, video conferencing will be used)

For questions on course content and assignments, please visit my office hours. Email is a good tool for inquiries concerning course logistics, etc, but it is not an efficient vehicle to discuss mathematics. Also keep in mind that email is a means of asynchronuous communication, i.e. immediate responses should not be expected. I will get to your email inquiries eventually.

Credit Weight: 0.5

Academic Department (or campus): Mathematics & Statistics

Campus: University of Guelph

Semester Offering: Fall 2021

3 Learning Resources

3.1 Lecture notes

Students are encouraged and expected to take their own notes during lectures. Written assignments will be an important part of the course that contain practice exercises and a more in depth treatment of some material. Assignments will be posted on courselink. An important resource will be be solutions to the assignment that will also be made available on courselink. The programming project will be posted on courselink in due time.

3.2 Textbooks

Required Texts: none

Recommended Texts: Many books cover the material of the course, all emphasising different aspects. Learners are encouraged to also inspect and consult additional texts. The first three on the following list are available as softcopy in pdf format from the library. The last two books were originally published by SIAM but we will use the below online versions.

- Stoer J, Bulirsch R. Introduction to Numerical Analysis, 3rd edition, Springer, 2002
- Allaire G, Kaber SM. Numerical Linear Algebra, Springer, 2008
- Björk A. Numerical Methods in Matrix Computations, Springer, 2015
- Y. Saad, Iterative methods for sparse linear systems, 2nd ed, http://www-users.cs.umn.edu/~saad/IterMethBook_2ndEd.pdf
- R. Barret et al, Templates for the solution of linear systems: Building blocks for iterative methods, www.netlib.org/templates/templates.pdf

3.3 Software

- GNU Fortran compiler (binaries and documentation): https://gcc.gnu.org/wiki/GFortran
- NVIDIA HPC Software Development Kit (SDK), contains the nvidia fortran compiler: https://developer.nvidia.com/hpc-sdk
- gnuplot visualisation software: http://www.gnuplot.info/
- programming editors with fortran syntax recognition include multipurpose software such as jedit (http://www.jedit.org/) and atom (https://atom.io/), but also some simpler general purpose editors will suffice (gedit, pluma, emacs, xemacs)

The first two items are compilers that are available free of charge. In class we will primarily use the gnu compiler, but it is always good to have a second compiler at hand during code development (for reasons we will discuss in class). The third item is a general purpose visualisation software for graphical postprocessing of numerical results. Finally you will need a text editor, e.g. one of the four listed in the last item, but others that you might feel more comfortable with are ok. Alternatively, you can also use an IDE, but when you submit your codes, keep in mind that I won't use the same IDE that you use and you will need to make sure to send me the source code files so that I can easily use them from command line.

3.4 Fortran Tutorials

Fortran will be introduced in class by discussing examples of increasing complexity. This will likely not be in sufficient detail to become a proficient programmer. Students will need to consult additional resources beyond that. Several tutorials are available that give an introduction to the programming language. I list here only a few:

- https://fortran-lang.org/learn/
- https://ourcodingclub.github.io/tutorials/fortran-intro/
- https://riptutorial.com/fortran

3.5 Additional resources may be announced in class

4 Learning Outcomes

General Learning Outcomes

1. Numeracy and quantitative skills
2. Critical and logical thinking
3. Application of mathematical knowledge
4. Independent learning of advanced mathematical concepts
5. Active and passive mathematical and scientific communication

Specific Learning Outcomes:

1. To increase the students computational literacy, both theoretically and practically
2. To improve algorithmic thinking
3. Students will be introduced to current numerical methods and learn about theoretical considerations to assess suitability, efficiency and accuracy of numerical approximations to unknown exact solutions
4. Students will gain hands-on experience using current computing technology to solve selected mathematical problems that arise frequently in mathematics and its application areas
5. Students will learn to design, implement, and test computational strategies for numerical problems

Lecture/project Content :

- review of direct linear solvers, vector norms and induced matrix norms
- floating point systems and computer arithmetics, errors, conditioning
- sparse matrix formats
- stationary iterative linear solvers
- Conjugate Gradient method and its extension to more general Krylov subspace solvers
- iterative nonlinear solvers (programming project)
- Fortran programming (programming project, assignments)
- data visualisation and animation (programming project)

5 Teaching and Learning Activities

Method of instruction

The main thrust of the course follows a traditional lecture model (delivered remotely and synchronuously) and include written assignments to practise and apply the material covered in the lectures. Students are expected to take their own notes during lectures. In the final weeks of the semester, students will work on a major project. The class will meet during this time regularly (during scheduled class hours) for Q&A, and additional ad hoc lectures accompanying the project.

Students should expect to spend 10-12 hrs/wk for their course work (including lectures).

6 Assessments

6.1 Marking Schemes & Distributions

Final grades will be determined based on the following:

Three written assignments in which the students will practise applying the concepts covered in class. The assignments should be written using professional language and style and provide sufficient explanation and detail of the rationale on which the answers/solutions are based. Each assignment will have at least one programming component.

A final exam will be held as a 25 minute long individually scheduled oral examination, reviewing the material of the course.

A course project will be carried out in the last phase of the term where students will individually work on a task that requires the use of methods discussed in the lecture. The project phase will be accompanied by Q&As during scheduled lecture hours and additional lectures specific to the project.

6.2 Assessment Details

Written assignments will be distributed at least one week before the due date, solutions will be posted after they have been marked:

Assignment 1 **(10%)**, due October 4
Assignment 2 **(10%)**, due October 18
Assignment 3 **(10%)**, due November 8

Final project (35%): will be posted in class in the second half of October with a due date on December 8.

Final examination (35%): The Final Exam will be an oral exam of 25min per student. By default, these exams will take place on WED Dec 15, 9:30-16:00, or at another time that week, as mutually agreed by instructor and student. The final exam will be held by zoom and recorded.

Grades and interpretation of grades. The normal grading system that is in use by the university applies, based on letter grade and percentage grades. The interpretation of grades is described in detail in the academic calendar.

7. General Statements

7.1 E-mail Communication

As per university regulations, all students are required to check their <uoguelph.ca> e-mail account regularly: e-mail is the official route of communication between the University and its students.

7.2 When You Cannot Meet a Course Requirement

When you find yourself unable to meet an in-course requirement because of illness or compassionate reasons, please advise the course instructor (or designated person, such as a teaching assistant) in writing, with your name, id#, and e-mail contact. See the undergraduate calendar for information on regulations and procedures for Academic Consideration.

7.3 Drop Date

Courses that are one semester long must be dropped by the end of the last day of classes; two-semester courses must be dropped by the last day of classes in the second semester. The regulations and procedures for Dropping Courses are available in the Undergraduate Calendar.

7.4 Copies of out-of-class assignments
Keep paper and/or other reliable back-up copies of all out-of-class assignments: you may be asked to resubmit work at any time.

7.5 Accessibility
The University promotes the full participation of students who experience disabilities in their academic programs. To that end, the provision of academic accommodation is a shared responsibility between the University and the student.

When accommodations are needed, the student is required to first register with Student Accessibility Services (SAS). Documentation to substantiate the existence of a disability is required, however, interim accommodations may be possible while that process is underway.

Accommodations are available for both permanent and temporary disabilities. It should be noted that common illnesses such as a cold or the flu do not constitute a disability.

Use of the SAS Exam Centre requires students to make a booking at least 7 days in advance, and no later than November 1 (fall), March 1 (winter) or July 1 (summer). Similarly, new or changed accommodations for online quizzes, tests and exams must be approved at least a week ahead of time.

More information: www.uoguelph.ca/sas

7.6 Academic Misconduct

The University of Guelph is committed to upholding the highest standards of academic integrity and it is the responsibility of all members of the University community – faculty, staff, and students – to be aware of what constitutes academic misconduct and to do as much as possible to prevent academic offences from occurring. University of Guelph students have the responsibility of abiding by the University's policy on academic misconduct regardless of their location of study; faculty, staff and students have the responsibility of supporting an environment that discourages misconduct. Students need to remain aware that instructors have access to and the right to use electronic and other means of detection.

Please note: Whether or not a student intended to commit academic misconduct is not relevant for a finding of guilt. Hurried or careless submission of assignments does not excuse students from responsibility for verifying the academic integrity of their work before submitting it. Students who are in any doubt as to whether an action on their part could be construed as an academic offence should consult with a faculty member or faculty advisor.

Graduate Calendar - Academic Misconduct

https://www.uoguelph.ca/registrar/calendars/graduate/current/genreg/index.shtml

7.8 Recording of Materials

Presentations which are made in relation to course work—including lectures—cannot be recorded or copied without the permission of the presenter, whether the instructor, a classmate or guest lecturer. Material recorded with permission is restricted to use for that course unless further permission is granted.

7.9 Resources

The Academic Calendars are the source of information about the University of Guelph's procedures, policies and regulations which apply to undergraduate, graduate and diploma programs.

8. Additional University Statements

8.1 Online Behaviour

Inappropriate online behaviour will not be tolerated. Examples of inappropriate online behaviour include:

- Posting inflammatory messages about your instructor or fellow students
- Using obscene or offensive language online
- Copying or presenting someone else's work as your own
- Adapting information from the Internet without using proper citations or references

- Buying or selling term papers or assignments
- Posting or selling course materials to course notes websites
- Having someone else complete your quiz or completing a quiz for/with another student
- Stating false claims about lost quiz answers or other assignment submissions
- Threatening or harassing a student or instructor online
- Discriminating against fellow students, instructors and/or TAs
- Using the course website to promote profit-driven products or services
- Attempting to compromise the security or functionality of the learning management system
- Sharing your user name and password
- Recording lectures without the permission of the instructor

8.2 Recording of Lecture Materials

The University of Guelph's primary mode of course delivery has shifted from face-to-face instruction to remote and online learning due to the ongoing COVID-19 pandemic. As a result, some learning activities (e.g., synchronous lectures or student presentations) may be recorded by faculty, instructors and TAs and posted to CourseLink for grading and dissemination; students may be recorded during these sessions.

By enrolling in a course, unless explicitly stated and brought forward to their instructor, it is assumed that students agree to the possibility of being recorded during lecture, seminar or other "live" course activities, whether delivery is in-class or online/remote.

If a student prefers not to be distinguishable during a recording of a lecture, they may:

1. turn off their camera
2. mute their microphone (does not apply to the oral examination)
3. edit their name (e.g., initials only) upon entry to each session

Students who express to their instructor that they, or a reference to their name or person, do not wish to be recorded may discuss possible alternatives or accommodations with their instructor.

This does not apply to the oral exams, during which the student must be identifiable. Exams are recorded solely for later use in dispute resolution if the need arises.

8.3 Illness

Medical notes will not normally be required for singular instances of academic consideration, although students may be required to provide supporting documentation for multiple missed assessments or when involving a large part of a course (e.g.. final exam or major assignment).

8.4 Information on current safety protocols

Follow these links: https://news.uoguelph.ca/return-to-campuses/how-u-of-g-is-preparing-for-your-safe-return/ https://news.uoguelph.ca/return-to-campuses/spaces/#ClassroomSpaces

8.5 Mental Health Services:

One out of every five students in Canada experiences some sort of mental health issue at some point in their academic career. If you find yourself facing a mental health crisis, or just need to talk to someone, please consider taking advantage of one of the following resources available to University of Guelph students:

Counselling Services: Visit the Counselling Services website (https://wellness.uoguelph.ca/counselling) to get information on resources available to you, both online and in-person. You can also visit them at Health Services (J.T. Powell Building, ext 53244) where they offer individual and group counselling sessions by appointment or walk-in.

Student Support Network: is located in the Wellness & Education Promotion Centre in the J.T. Powell Building and offers confidential, peer-based, drop-in support.

Good2Talk: (1-866-925-5454) is a free, 24/7 student hotline that provides professional counselling and referrals for mental health, addictions and well-being.

Here 24/7: (1-844-437-3247) specializes in assessment, referral and appointment booking and is available 24/7 for crisis support.

You are not alone and you will not be judged for asking for help.