ChE 322 - Numerical Methods for Process Analysis and Design

Calendar Description:
Numerical Methods for Process Analysis and Design
Systems of linear and non-linear algebraic equations; polynomial and spline interpolation; numerical differentiation and integration; numerical solution of initial value and boundary value ordinary differential equation problems: accuracy and stability, step size control and stiffness; finite differences for the numerical solution of elliptic and parabolic partial differential equations: method of lines, explicit vs. implicit finite-difference methods; introduction to the finite element method (optional).
Prereq: 3A Chemical Engineering

Instructor:

Prof. A. Elkamel, PhD, PEng.
Office: E6 - 3008
Phone: (519) 888-4567 x37157
Email: I check my e-mail (aelkamel@uwaterloo.ca) almost daily and try to respond in a reasonable amount of time.
Official Office Hours: Mondays [11:30 a.m. – 12:50 p.m.] or [by appointment through Microsoft Teams]

Official Office Hours:
Wednesdays - 11:20 a.m. – 12:30 p.m. or
Fridays - 4:30– 5:30 p.m. or [by appointment]

Teaching Assistant: Abhishek Yogesh Gandhi
Email: aygandhi@uwaterloo.ca
Official Office Hours: by appointment

Scheduled Sessions:

Lectures:

Mondays	[9:30 a.m. - 11:20 a.m.]	DWE - 2529
Wednesdays	[4:30 p.m. - 5:20 p.m.]	DWE - 2529

Tutorials:

Wednesdays	[3:30 p.m. - 4:20 p.m.]	DWE – 2529

to be conducted by Teaching Assistant

Tutorials: Tutorials will be posted with solutions after the tutorial session.
During the first week of classes, the tutorial session will be substituted with a lecture. Also, the lecture scheduled for June 26 (week of exam) will serve as a tutorial review instead.

Online Communication:
I will be making frequent use of UW-LEARN and I will be sending e-mails quite often to the class. So make sure you make a habit out of checking UW-LEARN and your e-mail.

Course Reference Material:
Textbook (optional): "Applied Numerical Methods with Python", Steven C. Chapra and David E. Clough, McGraw-Hill Book Company (any edition!!).

Other Useful References:

1. "Applied Numerical Methods for Scientists and Engineers", S. Rao, Printice Hall.
2. "Numerical Methods for Engineers and Scientists" (1993), Joe Hoffman, McGraw-Hill Book Company.
3. "Numerical Methods for Engineers" (1996), Bilal Ayyub and Richard McCuen, Printice Hall
4. "Numerical Methods Using MATLAB" (1995), G. Lindfield and J. Penny, Ellis Horwood.
5. "MATLAB for Engineers" (1995), Adrian Biran and Moshe Breiner, Addison-Wesley.
6. "Numerical Methods for Chemical Engineers with MATLAB Applications", Alkis Constantinides and Navid Mostoufi, Printice Hall
7. "An Introduction to Numerical Methods for Chemical Engineers", James B. Riggs, Texas Tech University Press.
8. "Applied Numerical Methods for Engineers", Robert J. Schilling and Sandra L. Harris, Brooks/Cole.
9. P. Gries, J. Campbell, J. Montojo. Practical Programming: An Introduction to Computer Science Using Python 3.6 (2017) O'Reilly and Associates, Inc.
10. A. B. Downey, A. B. Think Python (2012) O'Reilly Media, Inc.

Knowledge, Abilities and Skills Students Should Gain in this Course:

At the end of this course, the student should

1. Describe mathematical algorithms for a range of common problems of chemical engineering interest (including root finding, systems of simultaneous equations, interpolation, differentiation and integration, and ordinary and partial differential equations).
2. Describe related numerical concepts, such as types of error, stability, convergence.
3. Apply Taylor Series expansion to determine the order of truncation error for a given algorithm.
4. Design and implement a simple computer program towards a specified mathematical algorithm using Python and evaluate the output of the program (including debugging).
5. Apply numerical methods to the solution of chemical engineering problems.

Lecture Topics

1 Course Introduction, Mathematical Modeling, Numerical Methods
2 Roots of equations
3 Systems of Nonlinear Equations
4 Systems of Linear equations
5 Curve Fitting and Interpolation
6 Numerical Integration
7 Numerical Differentiation
8 Ordinary differential equations (initial value problems)
9 Ordinary differential equations (boundary value problems)
10 Partial differential equations (elliptical equations)
11 Partial differential equations (parabolic equations)
12 Partial differential equations (method of lines)
13 Optimization (if time permits)

Homework:
Homework is an essential element in learning the type of material being taught in this course. There will be six assignments, roughly one every two weeks. Homework assignments will not be collected. Instead, five or six quizzes will be given. All HW solutions will be posted on the course web site.

Reading Assignments:
For each lecture you should plan to spend two hours reading your notes, handouts, and books. The best time to study is the same day as the lecture, so that no unclear points remain. Not keeping up is a sure way of failing to meet the course objectives.

Exams and Quizzes:

All exams will be closed books, closed notes, unless otherwise indicated. Remember that according to university regulations the penalty for dishonesty is severe: at least failure of the course (not just the exam). Make-up exams will not be given. Any student who cannot take an exam as scheduled must make special arrangements with Dr. Elkamel before the exam is given.

A one hour and 30 minutes (from 3:30 p.m. – 5:00 p.m.) midterm exam will be given on June 28, 2023. This will be through the Learn environment.

The final exam will cover all material in the course, including any new material since the last quiz. The time and place will be announced by the registrar.

Course Grading:

Quizzes	:	10%
Project	:	10%
Midterm	:	30%
Final	:	50%

Grades will be assigned on the basis of the final class average. I do not use a predetermined scale.

In grading quizzes and examinations, the emphasis will be on a correct approach to the problem. A numerically correct answer derived from an unsound approach will receive little credit.

Project: A major component of the course requirements is a term project. The goal of the project is to allow you to apply the skills learned in this class in a way that is more closely related to actual engineering practice than homework or exam. You have more time to complete the project and have access to more resources than on an exam, but the scope of work is also greater and the expectations are higher.

The project is a joint project for CHE312 and CHE322. You will develop and solve a mathematical model for a heat transfer problem. The development of the model as well as the communication will be marked by Dr. Hamid Reza Kariminia Hamedaani and will account for 10% of your CHE312 course grade. The numerical solution and design considerations will be marked by Dr. Elkamel and will account for 10% of your CHE322 course grade. More details and a rubric will be provided.

Guiding Principles:
I consider the classroom to be a place where we all will be treated with respect. I welcome individuals of all ages, backgrounds, beliefs, ethnicities, genders, gender identities, gender expressions, national origins, religious affiliations, sexual orientations, ability – and other visible and nonvisible differences. All members of this class are expected to contribute to a respectful, welcoming and inclusive environment for every other member of the class.

LEARN: Course slides and other course materials will be posted on LEARN. Students are allowed and encouraged to download materials for their own personal files but are not authorized to post CHE322 materials on sites other than LEARN. Course deliverables will be available and submitted using LEARN.
Email Policy: Microsoft Teams or email is the best way to get in touch with the instructor. When sending an email, remember the following:
1. Emails should be sent from your official University of Waterloo email account.
2. Put CHE322 in the email subject line followed by a brief description of the email subject. For example, “CHE322: Question concerning Quiz 1”.
3. Sign your email with your first and last name and your student number.
4. Emails should contain professional and respectful language.
5. While we will do our best to respond to your emails as soon as possible, allow 24 to 48 hours (excluding weekends) for a response to your email.
6. If your question or concern requires a complex answer or warrants a discussion, the instructor may suggest a video meeting through Microsoft Teams.

Land Acknowledgement:
The University of Waterloo acknowledges that much of our work takes place on the traditional territory of the Neutral, Anishinaabeg and Haudenosaunee peoples. Our main campus is situated

on the Haldimand Tract, the land granted to the Six Nations that includes six miles on each side of the Grand River. Our active work toward reconciliation takes place across our campuses through research, learning, teaching, and community building, and is centralized within the Office of Indigenous Relations.

Religious Holidays: Students have the right to practice the religion of their choice. If you need to miss class to observe a religious holiday, please submit the dates of absence to the instructor by the end of the second full week of classes. The instructor will work with you to develop a mutually agreeable plan to make-up for missed class time and course work.

Academic integrity: In order to maintain a culture of academic integrity, members of the University of Waterloo community are expected to promote honesty, trust, fairness, respect and responsibility. [Check the Office of Academic Integrity for more information.]

Grievance: A student who believes that a decision affecting some aspect of his/her university life has been unfair or unreasonable may have grounds for initiating a grievance. Read Policy 70, Student Petitions and Grievances, Section 4. When in doubt, please be certain to contact the department's administrative assistant who will provide further assistance.

Discipline: A student is expected to know what constitutes academic integrity to avoid committing an academic offence, and to take responsibility for his/her actions. [Check the Office of Academic Integrity for more information.] A student who is unsure whether an action constitutes an offence, or who needs help in learning how to avoid offences (e.g., plagiarism, cheating) or about "rules" for group work/collaboration should seek guidance from the course instructor, academic advisor, or the undergraduate associate dean. For information on categories of offences and types of penalties, students should refer to Policy 71, Student Discipline. For typical penalties, check Guidelines for the Assessment of Penalties.

Appeals: A decision made or penalty imposed under Policy 70, Student Petitions and Grievances (other than a petition) or Policy 71, Student Discipline may be appealed if there is a ground. A student who believes he/she has a ground for an appeal should refer to Policy 72, Student Appeals.

Note for students with disabilities: AccessAbility Services, located in Needles Hall, Room 1401, collaborates with all academic departments to arrange appropriate accommodations for students with disabilities without compromising the academic integrity of the curriculum. If you require academic accommodations to lessen the impact of your disability, please register with AccessAbility Services at the beginning of each academic term.

COVID-19 Considerations.: There could be a need to make alternate arrangements for in-person course activities. This alternate arrangement could be for a short period of time (e.g., one week) or a more sustained disruption to in-person course activities. In the event of a disruption, all in-person lectures will revert to synchronous, online lectures.

If presentations are impacted, the most likely scenario is that these presentations will still occur but in a virtual format using MS Team meetings.

If you are unable to attend an in-person course activity due to emergency self-isolation, please let Professor Elkamel know as soon as possible (see COIVD-19-Related and Short-Term Absences below). If this will impact more than one course, you are encouraged to inform the Associate Chair Undergraduate Studies. They will review your case and coordinate a reasonable and fair plan in consultation with appropriate others.

Please also see 'Fair Contingencies for Remote Teaching' below and 'Instructional Contingencies for Covid-19' in the next section.

COVID-19-Related Absences and Short-Term Absences: If you declare a COVID-19-related two-day absence or short-term two (2) day absence and you will miss a graded component in CHE322, you need to reach out to Professor Ali Elkamel as soon as possible. It is expected that only individual deliverables will be eligible for accommodation unless there are extenuating circumstances like the vast majority of a team being on an absence at the same time.

INSTRUCTOR ABSENCES

If I am unable to come to campus but am well enough to teach, I will hold lecture remotely at the regularly scheduled time. You will be notified by email and on LEARN of these arrangements. If I am unable to teach, asynchronous online content will be provided.

Fair Contingencies for Remote Teaching: We are facing unusual and challenging times. The course outline presents the instructor's intentions for course assessments, their weights, and due dates in Spring 2023. As best as possible, we will keep to the specified assessments, weights, and dates. To provide contingency for unforeseen circumstances, the instructor reserves the right to modify course topics and/or assessments and/or weight and/or deadlines with due and fair notice to students. In the event of such challenges, the instructor will work with the Department/Faculty to find reasonable and fair solutions that respect the rights and workloads of students, staff, and faculty.

Turnitin.com: Text matching software (Turnitin®) may be used to screen assignments in this course. Turnitin® is used to verify that all materials and sources in assignments are documented. Students' submissions are stored on a U.S. server, therefore students must be given an alternative (e.g., scaffolded assignment or annotated bibliography), if they are concerned about their privacy and/or security. Students will be given due notice, in the first week of the term and/or at the time assignment details are provided, about arrangements and alternatives for the use of Turnitin in this course.

It is the responsibility of the student to notify the instructor if they, in the first week of term or at the time assignment details are provided, wish to submit the alternate assignment.

Writing and Communication Centre:

The Writing and Communication Centre works with students in all Faculties to help you consider your audience, clarify your ideas, develop your voice, and write in the style appropriate to your discipline. We offer one-on-one support for writing papers, delivering presentations, integrating research, and revising for clarity and coherence. Group appointments for team-based projects, presentations, and papers are also available.
All of our services are available virtually: booked appointments, drop-ins, resources, and writing groups. Check out our website for other ways to interact with us, such as open online forums and online "Question and Answers". Visit us at www.uwaterloo.ca/wcc.
Please note that communication specialists guide you to see your work as readers would. We can teach you revising skills and strategies, but will not change or correct your work for you. Please bring your assignment instructions and any notes or drafts to your appointment.
[Link **Writing and Communication Centre**]

Course and Departmental Expectations

Guiding Principles for our CHE Community (faculty, staff, and students): 1) Be compassionate. 2) Be accountable. 3) Be patient. 4) Be safe and healthy.

Compassionate and respectful communication: Most online communication between the Department and students will be done through LEARN and/or email. Students are reminded that they should now use their email account name@uwaterloo.ca. Include an academic signature with your full name, program, student ID. We encourage you to include your preferred pronouns (he/him; she/her; they/them).

Student Absences: There are many reasons a student may miss class due to illness, quarantining, isolation, vaccination side effects – we have been advised to handle these as we would have for a 2-week absence in the pre-COVID times. Guidelines are available in the undergraduate calendar. [Link Academic Accommodations due to illness]

Instructional Contingencies for Covid-19: Should we be required to move away from full-occupancy in-person teaching, the instructors will work with the Department to ensure that students have a fair opportunity to meet course requirements and to be notified of any changes in a timely manner.

CHE Comment on Accommodation: We respect that our CHE students are independent adult decision-makers, with many opportunities to partake in activities that might be in time conflict with academic deadlines and deliverables. Along with the right to make adult decisions comes the responsibility and accountability for those decisions and any outcomes.
The University of Waterloo's policy on accommodation for missed deliverables pertains to verifiable health matters, and highly unfortunate events (for example: family tragedies). The Department of Systems Design Engineering follows University of Waterloo's general policy: students who self-elect to forgo a deliverable receive a "0" for that deliverable. It is preferred practice so that fairness is maintained for members of the same class/course by avoiding preferential treatment, and so that instructors are not burdened with having to create extra quizzes, deliverables, etc. It also reflects professional practice, as failing to show up to work and missing deadlines can be very costly to the company and individual (for example: not submitting a contract proposal, or design review on time). ***Please read the policy here:*** [Link Accommodation due to illness]

CHE Academic Priorities over Co-op Interviews: Academic deliverables are to take priority over co-op interviews. This is especially true for course midterms and final exams. Students who have been scheduled for an interview at the same time as a course test, midterm, or exam MUST follow the CECA procedure for rescheduling the interview: [Link CECA rescheduling co-op interviews]

Compassionate Accommodation: If you are facing challenges that are affecting more than one course contact the Associate Chair Undergraduate Studies. They will review your case and coordinate a reasonable and fair plan in consultation with appropriate others (for example:

instructors, Department Undergraduate Studies Committee, Chair, AccessAbility Services, Engineering Counselling services, Registrar's Office).

FACULTY OF ENGINEERING – MORE FINE PRINT

Faculty of Engineering website: [Link Academic Support and Policies].

Academic Integrity: In order to maintain a culture of academic integrity, members of the University of Waterloo community are expected to promote honesty, trust, fairness, respect, and responsibility.
[Check Academic Integrity website for more information. Link Office of Academic Integrity].

Discipline: A student is expected to know what constitutes academic integrity (see link above) to avoid committing an academic offence, and to take responsibility for their actions. A student who is unsure whether an action constitutes an offence, or who needs help in learning how to avoid offences (for example: plagiarism, cheating) or about expectations for group work/collaboration should seek guidance from the course instructor, academic advisor, or the undergraduate Associate Dean. Relevant documents include:

- University of Waterloo Policy 71 [Link Policy 71 Student Discipline].
- Academic Penalty Guidelines [Link Policy 71 Penalty Guidelines].
- Assessment of Unauthorized Collaboration: [Link Assessment of Unauthorized Collaboration].

Grievance: A student who believes that a decision affecting some aspect of their university life has been unfair or unreasonable may have grounds for initiating a grievance. Read Policy 70, Student Petitions and Grievances, Section 4. When in doubt please be certain to contact the **Associate Chair Undergraduate or Academic Advisor** who will provide further assistance.
[Link Policy 70 Petitions & Grievance.]

Appeals: A decision made, or penalty imposed under Policy 70 (Student Petitions and Grievances) (other than a petition) or Policy 71 (Student Discipline) may be appealed if there is a ground. A student who believes they have a ground for an appeal should refer to Policy 72 (Student Appeals)
[Link Policy 72 Student Appeals].

AccessAbility Services: AccessAbility Services (A.A.S.) is the University's centralized office for the provision of academic accommodations for students with a known or unknown disability, illness, or condition. Even if students are unsure of whether they qualify for A.A.S. support, an A.A.S. consultant can talk them through next steps, and refer them elsewhere if appropriate.
[Link AccessAbility Services].