Chemical Engineering 2E04

Numerical Methods and Computing for Chemical Engineers

Course Outline - Fall 2023

Course Details

Instructor:		**Dr. Jake Nease**	**neasej@mcmaster.ca** **(905) 599-3165**	**BSB/B105**
Teaching Assistants:		Sagnik Guhathakurta	guhaths@mcmaster.ca	See A2L
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Website:		Avenue2Learn	avenue.mcmaster.ca	
Lectures*:		See A2L	See A2L	See A2L
Tutorials/Labs*:		See A2L		
Office Hours:	**INST:**	Monday	10:30 – 12:30 or **drop in**	
	TA:	Recitation and MP consultation Hours to be determined.		
Prerequisites:	Registration in Chemical Engineering or Materials Engineering, MATH 1ZA3/B3/C3			
Course Materials:	Lecture modules, tutorials, mastery problems, videos, and solutions will be posted on A2L Grades will be posted on A2L but are not official until released on MOSAIC.			
Recommended Textbook:	A. Gilat, V. Subramaniam: *Numerical Methods for Engineers and Scientists.* Wiley. Third Edition (2014): Wiley E-Book Campus Book Store			

*Based on University inclusion and safety policies, this information is available separately on Avenue to Learn.

Formal Course Description

Chemical Engineering 2E04 focuses on the formulation and solution of various engineering problems. We review a variety of techniques for numerical solution of linear and nonlinear model equations, including algebraic and ordinary differential equations, and the use of curve-fitting and interpolation methods.

Informal Course Description

A course dedicated to solving **hard problems** by approximating them as a ***bunch of easier problems*** solved efficiently and with high precision to minimize the errors introduced via simplification.

Learning Objectives

After completing this course, the student should be able to:

L.1. Recognize when numerical methods should be applied as a part of a solution to a variety of chemical engineering (and other) problems or opportunities.

L.2. Formulate mathematical models of common engineering unit operations and processes.

L.3. Identify the appropriate algorithm or numerical method suitable for the solution.

L.4. Break down how an algorithm works based on fundamental mathematical concepts.

L.5. Implement algorithms using calculators and (more importantly) software tools.

L.6. Derive algorithms for new problems based on a fundamental understanding of the objective.

L.7. Use a numerical solution to help solve the original problem of interest.

L.8. Identify the critical differences, advantages, and disadvantages of numerical versus analytical techniques.

Evidence of Objectives

Evidence to prove that one has achieved the above objectives may be demonstrated by:

- Explaining to a peer the fundamental concepts which are used in an algorithm.
- Using graphs and tables to illustrate how an algorithm works.
- Deriving potential algorithms to solve a problem from fundamental concepts.
- Coding an algorithm in a software tool such as `MATLAB` and proving that it works.
- Executing part of an algorithm "by hand" to show an understanding of core applied mathematics.
- Suggesting alternative algorithms for previously unsolved problems.
- Implementing the results of an algorithm in the final solution of the original problem.
- Explaining the importance of solving a problem (with or without numerical methods) in the first place.

Grading Policies

Please be aware of the following grading policies for ChE 2E04:

- Mastery problems have flexible due dates and therefore cannot be the subject of an MSAF.
- Valid MSAF submissions for midterms will result in either a make-up examination or rolling of that component's weight into the final exam, depending on the situation. The lab exam cannot be transferred.
- All assessments in this course are open-book (any book) and open-notes (any hard copies).
- Any calculator, but not computers, may be used for in-person written examinations.
- The instructor retains the right to modify course weights or components; this is typically only enforced for the student's benefit. All grades are **unofficial** until final grades are posted on MOSAIC.
- Final grades will be converted to the standard McMaster 12-point scale.
- All submissions for mastery problems and take-home examinations must be done **electronically**.
- Any copying of code, formulations, or interpretations from other students, prior versions of this course, or resources online will be considered a violation of McMaster's academic integrity policy.

Grading Breakdown

Weight	Component	Comments
0%	Tutorial Activities	Are there for your benefit and practice. Do them in groups!
12-39%	Mastery Problems	Individual or groups of 2. You MUST complete **four** for 12%. See MP Schedule. Additional problems displace lab exam (up to 27%).
25%	Midterm Tests	Two midterms, with in-class re-writes. Best is worth 15%, worst 10%.
28%	Written Exam	Individual written exam scheduled during the exam break.
3-30%	Lab Exam	Individual exam on computing. Value depends on mastery problems.
5%	Participation	Attendance in tutorial sessions (0.5% each, up to 10 sessions count)

Mastery Problems

Mastery problems are real-world applications of numerical methods and computing applied to engineering problems. These problems have been curated to expose students to the power of numerical computing while also allowing for a low-risk method to earn credit for computing work. A brief description is as follows:

- Mastery problems must be completed individually or in pairs.
    - Each problem is graded as **successful/unsuccessful**.
    - You may submit each problem **as many times as you want** before the due date.
    - You can book **office hours** with the instructor and TAs to help you and receive feedback.
    - You choose your own pairs and may submit each problem with a different partner if you wish.
- Each problem is **worth 3%** of your final grade.
    - You MUST complete one problem from chapters 1-4 of the course (12%)
    - After completing one problem, each other from that chapter displace 3% from the lab exam.
    - Completing all mastery problems results in a lab exam worth 3%.
    - Academic dishonesty on mastery problems will result on **0% on the weight of mandatory problems and reversion to a 30% lab exam. No exceptions.**
- Mastery problems must be submitted **electronically** via the appropriate A2L drop box.
    - **Only one** group member should submit the problem.
    - Pay attention to the submission guidelines on the front page of each problem.
    - Ensure your submission outputs the deliverables required at the end of each problem.
    - You may re-submit any problem any number of times. The drop boxes for optional problems close at 11:59pm Dec 6.
- Mastery problems will be graded **twice per week**. You will only know your result at those times. Plan accordingly!

Lab Examination

The lab examination is initially worth 30% of your final grade. As discussed above, successfully completing mastery problems throughout the term beyond the minimum of four shifts 3% of the lab exam to that mastery problem. It is possible to have a lab exam worth 3%. You may continue to submit mastery problems AFTER the lab exam is complete.

Academic Honesty

You are expected to exhibit honesty and use ethical behaviour in all aspects of the learning process. Academic credentials you earn are rooted in principles of honesty and academic integrity.

Academic dishonesty is to knowingly act or fail to act in a way that results or could result in unearned academic credit or advantage. This behaviour can result in serious consequences, *e.g.* the grade of zero on an assignment, loss of credit with a notation on the transcript (notation reads: "Grade of F assigned for academic dishonesty"), and/or suspension or expulsion from the university. **Note that these consequences will be enforced even when submitting OPTIONAL components**. It is your responsibility to understand what constitutes academic dishonesty. For information on the various types of academic dishonesty please refer to the Academic Integrity Policy, located at http://www.mcmaster.ca/academicintegrity.

- All mastery problems **are to be done individually or in your pairing only**, with no additional collaboration. I will facilitate discussion boards to allow you to help each other out.
- Tutorials will not be marked. Feel free to work in groups or get outside help. They are for your understanding and skill development. If you work better alone, do it alone.
- Plagiarism, improper collaboration, copying unauthorized tests or aids, and other academic dishonesty will not be tolerated. **Your first offence will be reported** to the Office of Academic Integrity.
- The default penalty for academic dishonesty is a zero on the entire problem / assignment / exam, even if the dishonesty occurred on just one portion or question of that problem/ assignment / exam. However, if Academic Integrity chooses to hold a hearing, they will determine the penalty.

Accessibility and Mental Health

The instructor aims to make this class accessible to all students. Please forward and optionally discuss any accommodation granted by Student Accessibility Services (SAS) with the instructor *before the third week of the course*. Please raise any other accessibility issues with the instructor as soon as possible, *e.g.* accessibility of the course website and course materials.

I am certified with the McMaster Professor Hippo on Campus Program for mental health awareness and aid to students in need. My office (or online video portal) is a **safe space** to discuss issues both academic and otherwise, and you are welcome to contact me at any time to chat. If I reach out to you at any time, be aware that it is not to embarrass or penalize you; it is because I care.

Course Feedback

Please do not hesitate to let me know your thoughts on the course or what you might want to change at any time. You can reach me at neasej@mcmaster.ca. If you would prefer to leave feedback **anonymously**, do not hesitate to use our anonymous 2E04 course feedback form.

Class Recordings

I am keenly aware that coming to class live is not always possible. Although I strongly recommend that you attend lectures and tutorials live, if you must miss for any reason, please note that all live lectures will be recorded.

Recordings will be done via ECHO360 lecture capture. I make no guarantees on quality or reliability of ECHO360, but hopefully everything works out great. Videos will be posted on our course YouTube channel weekly.

Class Coding Sessions

Quite frequently in this course we will be using our engineering knowledge and material covered in lecture to derive algorithms to achieve a variety of outcomes. Often, especially toward the beginning of the course, we will then code these algorithms together in class to see their implementation in real-time. Some of the codes will use pre-built functions or even previous codes we have developed! Mastery problems may also refer to these codes. **All in-class codes will be posted on A2L for you to use freely**.

Tutorials

Note that although tutorials are not graded, it is strongly recommended that students work through them at their own pace. Each tutorial (and mastery problem) contains important information relevant to the course and is fair game for assessment. Tutorial time may also be used to work on **mastery problems**, but the instructional team's time will be prioritized to helping students with the tutorial activities.

Important Dates

There are several important dates for this course. Please commit these to your calendar:

- Written Midterm 1 — October 17 @ 19:00 — PGCLL (124, B131)
- Written Midterm 2 — November 14 @ 19:00 — PGCLL (124, B131)
- Lab Exam — November 28 @ 18:30 — PGCLL (124, B131)
- Last day of classes — December 06

Anticipated Tutorial Breakdown

Week Number	Week Starting…	Tutorial Topic
Week 2	September 12	Solving basic problems with `MATLAB`
Week 3	September 19	Creating and using functions
Week 4	September 26	Precision and truncation errors
Week 5	October 03	Timing linear solver algorithms
Week 6	October 10	Intro to nonlinear systems
RW	*Reading Week*	*Suggestion: Dune (Frank Herbert)*
Week 7	October 25	Bisection and Regula Falsi
Week 8	November 01	Hybrid nonlinear open methods
Week 9	November 08	Polynomial regression
Week 10	November 15	Spline interpolation
Week 11	November 22	Numerical differentiation
Week 12	November 29	Numerical integration
Week 13*	December 5	ODE integration

** No scheduled tutorials this week – but the activity is available for your own practice.*

Assumed Knowledge and Getting Help

MATLAB is one of the key tools which you will learn to use in this course. MATLAB is both a programming language and a math tool. All chemical engineering students are required to complete both a programming course in their first year and use MATLAB in their second-year math courses. This course will aim to equip students to use MATLAB in the future and be more successful in their math courses.

This course is built assuming that students are at least familiar with concepts covered in first year, such as:

- Basic program flow
- Variables and memory
- IF statements
- FOR loops and WHILE loops
- Functions
- Basic data plotting

To help students, a variety of learning aids have been posted on the course website:

Recitations: Teaching assistants will lead optional weekly review sessions called Recitations where time will be devoted to the review of lecture or problem material.

Videos: ChE 2E04 has a YOUTUBE channel!
Numerical Methods ChE McMaster

- Ep 1: Intro and Basics
- Ep 2: Matrices and Matrix Math
- Ep 3: For Loops and Pretty Graphs
- Ep 4: Functions! Functions! Functions!
- Ep 5: While loops, If Statements, & Breakpoints

Computation Guides: Supplementary information to help better understand concepts in programming and numerical methods. Again, these have been generously provided by Dr. Adams from his years of experience with 2E04. These guides can be found on the course website as well.

Guide 1: Computational Complexity

Guide 2: Thinking like a Computer

Guide 3: Variable Scope

Other McMaster MATLAB Guides:

Guide 1: MATLAB Primer written by a former McMaster prof

Guide 2: MATLAB Presentation written by former graduate students

Guide 3: Making Friends with MATLAB (Module 0) developed by our own 2E04 student team

Anticipated Course Schedule and Topics

Below is an outline of the topics I hope to cover in this course. This schedule is subject to change, especially in the early-goings as we get our bearings around MATLAB. *Topics in italics are only going to be covered if the pace of the class permits*. Note that each module is expected to take (roughly) 1-2 weeks, depending on size.

Module	Primary Module Topics	Content (subject to change)
Module 01A	Course Overview Linear Systems of Equations	• Overview of course structure • Linear system modeling • Language and lingo • Expansion to discretized systems
Module 01B	Linear System Solutions: Elimination Methods	• Gauss elimination • Gauss-Jordan elimination • LU decomposition • Trade-Offs and applications • Pivoting
Module 01C	Linear System Solutions: Iterative Methods	• Jacobi method • Gauss-Seidel method • Diagonal dominance • Smoothing • Condition numbers
Module 02A	Nonlinear Systems: Formulation and Bracketing	• Formulating nonlinear problems • Bisection for univariate solutions • Regula-Falsi for univariate equations • Rates of convergence
Module 02B	Nonlinear Systems: Open Methods and Multivariate Solutions	• Secant method • Review: Taylor Series expansion • Newton-Raphson method • Multivariate Newton-Raphson method
Module 03A	Curve Fitting: Regression	• Concept of regression and optimization • Linear regression • Polynomial regression • Basis function regression
Module 03B	Curve Fitting: Interpolation	• *Lagrange polynomials* • *Splines* • Data scaling and normalization
Module 04A	Numerical Differentiation	• Finite differences • Partial derivatives • *Derivatives via curve fitting* • Error analysis
Module 04B	Numerical Integration	• Newton-Cotes formulas and error analysis • Richardson extrapolation • *Romberg integration* • *Multiple integrals*
Module 05A	Univariate Differential Equations	• Defining ODEs • Methods of solving ODEs
Module 05B	Multivariate Differential Equations	• *Multivariate Euler's, and RK4 methods*

C.E.A.B. Graduate Attributes

Certain courses in the chemical engineering curriculum collect indicator data related to the development of the attributes deemed critical for engineers according to the Canadian Engineering Accreditation Board (CEAB). These indicators will be assessed throughout the course and redacted samples of student work may be collected for submission to the CEAB during McMaster Engineering's accreditation cycle. The indicators assessed in ChE 2E04 are as follows:

1.1 – Competence in mathematics.
1.3 – Competence in engineering fundamentals.
5.1 – Evaluates engineering tools, identifies their limitations, and selects, adapts, or extends them appropriately.
5.2 – Successfully uses engineering tools.
7.1 – Demonstrates comprehension of technical and non-technical instructions and questions.

The CEAB indicators listed above are mapped to the course learning outcomes as shown in the table at right. The CEAB accreditation process is an important component to curriculum design in engineering. If you have any questions or wish to be involved in the accreditation process, please let me know at neasej@mcmaster.ca.

Indicator	Mapped Learning Outcomes
1.1	L.2 L.4 L.5
1.3	L.1 L.2 L.3 L.7 L.8
5.1	L.3 L.4 L.6 L.8
5.2	L.3 L.5
7.1	L.1 L.7 L.8

The P.R.O.C.E.S.S.

The department of Chemical Engineering has a storied history of education. In addition to teaching and learning, the department is proud of our graduates not only for their academic success, but their more intrinsic traits that make them respected members of the engineering community.

Recently, several high-ranking graduates from the McMaster Chemical Engineering Program employed in various industries (oil/gas, financials, *etc*.) were interviewed to ask what traits they look for when hiring for engineering positions. Using this information, the department would like to present to you the **PROCESS**: a code of conduct that we hope will guide our students throughout this program and their careers to come.

- **P**rofessionalism
- **R**esponsibility
- **O**wnership
- **C**uriosity
- **E**mpathy
- **S**elflessness
- **S**ervice

It is up to YOU to interpret these traits and apply them to your time at McMaster and your career as you see fit. These traits will not be assessed for grades but will be strongly encouraged throughout your time at McMaster. We hope that you identify with these character traits and what they mean to you, and that you **trust the process**.

McMASTER APPROVED ADVISORY STATEMENTS

Authenticity / Plagiarism

Some courses may use a web-based service (Turnitin.com) to reveal authenticity and ownership of student submitted work. For courses using such software, students will be expected to submit their work electronically either directly to Turnitin.com or via an online learning platform (e.g. Avenue to Learn, etc.) using plagiarism detection (a service supported by Turnitin.com) so it can be checked for academic dishonesty.

Students who do not wish their work to be submitted through the plagiarism detection software must inform the Instructor before the assignment is due. No penalty will be assigned to a student who does not submit work to the plagiarism detection software. **All submitted work is subject to normal verification that standards of academic integrity have been upheld** (e.g., on-line search, other software, etc.). For more details about McMaster's use of Turnitin.com please go to www.mcmaster.ca/academicintegrity.

Courses with an On-line Element

Some courses may use on-line elements (e.g. e-mail, Avenue to Learn, LearnLink, web pages, capa, Moodle, ThinkingCap, etc.). Students should be aware that, when they access the electronic components of a course using these elements, private information such as first and last names, user names for the McMaster e-mail accounts, and program affiliation may become apparent to all other students in the same course. The available information is dependent on the technology used. Continuation in a course that uses on-line elements will be deemed consent to this disclosure. If you have any questions or concerns about such disclosure please discuss this with the course instructor.

Online Proctoring

Some courses may use online proctoring software for tests and exams. This software may require students to turn on their video camera, present identification, monitor and record their computer activities, and/or lock/restrict their browser or other applications/software during tests or exams. This software may be required to be installed before the test/exam begins.

Conduct Expectations

As a McMaster student, you have the right to experience, and the responsibility to demonstrate, respectful and dignified interactions within all of our living, learning and working communities. These expectations are described in the Code of Student Rights & Responsibilities (the "Code"). All students share the responsibility of maintaining a positive environment for the academic and personal growth of all McMaster community members, **whether in person or online.**

It is essential that students be mindful of their interactions online, as the Code remains in effect in virtual learning environments. The Code applies to any interactions that adversely affect, disrupt, or interfere with reasonable participation in University activities. Student disruptions or behaviours that interfere with university functions on online platforms (e.g. use of Avenue 2 Learn, WebEx or Zoom for delivery), will be taken very seriously and will be investigated. Outcomes may include restriction or removal of the involved students' access to these platforms.

Academic Accommodation of Students with Disabilities

Students with disabilities who require academic accommodation must contact Student Accessibility Services (SAS) at 905-525-9140 ext. 28652 or sas@mcmaster.ca to make arrangements with a Program Coordinator. For further information, consult McMaster University's Academic Accommodation of Students with Disabilities policy.

Requests for Relief for Missed Academic Term Work

In the event of an absence for medical or other reasons, students should review and follow the Policy on Requests for Relief for Missed Academic Term Work.

Academic Accommodation for Religious, Indigenous, or Spiritual Observances (RISO)

Students requiring academic accommodation based on religious, indigenous or spiritual observances should follow the procedures set out in the RISO policy. Students should submit their request to their Faculty Office ***normally within 10 working days*** of the beginning of term in which they anticipate a need for accommodation or to the Registrar's Office prior to their examinations. Students should also contact their instructors as soon as possible to make alternative arrangements for classes, assignments, and tests.

Copyright and Recording

Students are advised that lectures, demonstrations, performances, and any other course material provided by an instructor include copyright protected works. The Copyright Act and copyright law protect every original literary, dramatic, musical and artistic work, **including lectures** by University instructors.

The recording of lectures, tutorials, or other methods of instruction may occur during a course. Recording may be done by either the instructor for the purpose of authorized distribution, or by a student for the purpose of personal study. Students should be aware that their voice and/or image may be recorded by others during the class. Please speak with the instructor if this is a concern for you.

Extreme Circumstances

The University reserves the right to change the dates and deadlines for any or all courses in extreme circumstances (e.g., severe weather, labour disruptions, etc.). Changes will be communicated through regular McMaster communication channels, such as McMaster Daily News, Avenue to Learn and/or McMaster email.