McGill
Faculty of Engineering

Course Outline
CHEE 390

Course Title:	**Computational Methods in Chemical Engineering**
Credits:	**3**
Contact Hours:	**(3-1-5)**
Course Prerequisite(s):	**CHEE 204, COMP 208, MATH 263**
Course Corequisite(s):	**MATH 264**
Course Description:	**Linear systems of algebraic equations, Gaussian elimination; non-linear algebraic systems: Taylor series, incremental search, bisection method, linear interpolation, Newton-Raphson's method; differentiation and integration; initial value problems: Euler's and Runge Kutta's methods, stiff equations, adaptive solvers; boundary value problems; curve fitting; numerical optimization; probability theory and stochastic simulation: Monte Carlo method.**

Canadian Engineering Accreditation Board (CEAB) Curriculum Content

CEAB curriculum category content	Number of AU's	Description
Math	**23**	Mathematics include appropriate elements of linear algebra, differential and integral calculus, differential equations, probability, statistics, numerical analysis, and discrete mathematics.
Natural science		Natural science includes elements of physics and chemistry, as well as life sciences and earth sciences. The subjects are intended to impart an understanding of natural phenomena and relationships through the use of analytical and/or experimental techniques.
Complementary studies		Complementary studies include the following areas of study to complement the technical content of the curriculum: engineering economics; the impact of technology on society; subject matter that deals with central issues, methodologies, and thought processes of the arts, humanities and social sciences; management; oral and written communications; healthy and safety; professional ethics, equity and law; and sustainable development and environmental stewardship.
Engineering science	**23**	Engineering science involves the application of mathematics and natural science to practical problems. They may involve the development of mathematical or numerical techniques, modeling, simulation, and experimental procedures. Such subjects include, among others, applied aspects of strength of materials, fluid mechanics, thermodynamics, electrical and electronic circuits, soil mechanics, automatic control, aerodynamics, transport phenomena, elements of materials science, geoscience, computer science, and environmental science.
Engineering design		Engineering design integrates mathematics, natural sciences, engineering sciences, and complementary studies in order to develop elements, systems, and processes to meet specific needs. It is a creative, iterative, and open-ended process, subject to constraints which may be governed by standards or legislation to varying degrees depending upon the discipline. These constraints may also relate to economic, health, safety, environmental, societal or other interdisciplinary factors.

Accreditation units (AU's) are defined on an hourly basis for an activity which is granted academic credit and for which the associated number of hours corresponds to the actual contact time: one hour of lecture (corresponding to 50 minutes of activity) = 1 AU; one hour of laboratory or scheduled tutorial = 0.5 AU. Classes of other than the nominal 50-minute duration are treated proportionally. In assessing the time assigned to determine the AU's of various components of the curriculum, the actual instruction time exclusive of final examinations is used.

Graduate Attributes

This course contributes to the acquisition of graduate attributes as follows:

Graduate attribute	KB	PA	IN	DE	ET	IT	CS	PR	IE	EE	EP	LL
Level descriptor	D	D	n/a	n/a	n/a	D	n/a	n/a	n/a	n/a	n/a	n/a

n/a = Not applicable; I = Introduced; D = Developed; A = Applied

KB- *Knowledge Base for Engineering: Demonstrated competence in university level mathematics, natural sciences, engineering fundamentals, and specialized engineering knowledge appropriate to the program.*

PA *- Problem Analysis: An ability to use appropriate knowledge and skills to identify, formulate, analyze, and solve complex engineering problems in order to reach substantiated conclusions.*

IN *-Investigation: An ability to conduct investigations of complex problems by methods that include appropriate experiments, analysis and interpretation of data, and synthesis of information in order to reach valid conclusions.*

DE- *Design: An ability to design solutions for complex, open-ended engineering problems and to design systems, components or processes that meet specified needs with appropriate attention to health and safety risks, applicable standards, economic, environmental, cultural and societal considerations.*

ET- *Use of Engineering Tools: An ability to create, select, adapt, and extend appropriate techniques, resources, and modem engineering tools to a range of engineering activities, from simple to complex, with an understanding of the associated limitations.*

IT *-Individual and Team Work: An ability to work effectively as a member and leader in teams, preferably in a multi-disciplinary setting.*

CS- *Communication Skills: An ability to communicate complex engineering concepts within the profession and with society at large. Such abilities include reading, writing, speaking and listening, and the ability to comprehend and write effective reports and design documentation, and to give and effectively respond to clear instructions.*

PR *- Professionalism: An understanding of the roles and responsibilities of the professional engineer in society, especially the primary role of protection of the public and the public interest.*

IE *-Impact of Engineering on Society and the Environment: An ability to analyse social and environmental aspects of engineering activities. Such abilities include an understanding of the interactions that engineering has with the economic, social, health, safety, legal, and cultural aspects of society; the uncertainties in the prediction of such interactions; and the concepts of sustainable design and development and environmental stewardship.*

EE- *Ethics and Equity: An ability to apply professional ethics, accountability, and equity.*

EP- *Economics and Project Management: An ability to appropriately incorporate economics and business practices including project, risk and change management into the practice of engineering, and to understand their limitations.*

LL *- Life-Long Learning: An ability to identify and to address their own educational needs in a changing world, sufficiently to maintain their competence and contribute to the advancement of knowledge.*

Policies

Academic Integrity

McGill University values academic integrity. Therefore, all students must understand the meaning and consequences of cheating, plagiarism and other academic offences under the Code of Student Conduct and Disciplinary Procedures.
(see www.mcgill.ca/studentslsrrlhonestl for more information).
(approved by Senate on 29 January 2003)

In accord with McGill University's Charter of Students' Rights, students in this course have the right to submit in English or in French any written work that is to be graded.
(approved by Senate on 21 January 2009)

Grading Policy

In the Faculty of Engineering, letter grades are assigned according to the grading scheme adopted by the professor in charge of a particular course. This may not correspond to practices in other Faculty and Schools in the University.

In the event of extraordinary circumstances beyond the University's control, the content and/or evaluation scheme in this course is subject to change.

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CHEE 390 Computational Methods in Chemical Engineering

Fall 2017

Class Schedule

T & R 1:05-2:25, Wong 1020, Sep 5 – Dec 5

Instructor

Phillip Servio, PhD
Office: Wong 4110
Phone: 398-1026
Email: phillip.servio@mcgill.ca
Office hours: W 11:00-12:00 or by appointment

Teaching Assistants (TAs)

Olubukola Alimi (olubukola.alimi@mail.mcgill.ca)
Raymond Tran (raymond.tran@mail.mcgill.ca)
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Communication

My personal website (accessible via http://www.hydratetech.com/computational) will be used to distribute course materials, including lecture slides, reading assignments, and instructions for assignments & term project.

If you need to reach me, please send an email to phillip.servio@mcgill.ca. I will try to respond within 24-48 hours. If you have questions about the material, please come to my designated office hours or schedule an appointment. Specific questions about problems or theory will not be answered through email.

Course Description

This course is an introduction to computational methods, which attempts to unite the applications of numerical mathematics and scientific computing to real world chemical engineering problems. The student is assumed to have taken the introductory undergraduate classes in calculus and differential equations and to have some experience in computer programming. The course will focus on linear and non-linear algebraic systems, initial value problems, boundary value problems, probability and stochastic simulation, data fitting and regression, and numerical optimization. The benefits and limitations of each numerical method as well as the errors associated with each method will also be described. The techniques taught will be used to solve vapour-liquid and chemical reaction equilibria; heat, mass and momentum transfer; process simulation; chemical reactor design and optimization problems. The complexity of the problems will vary from one-dimensional and steady-state to multi-dimensional and transient. The student will also become familiar with the MATLAB® technical language, which will be used throughout the course in order to solve the problems.

Course Materials

There is no textbook for this course. All necessary material, e.g., lecture notes, readings, etc., will be posted on my website or given in class. Students will be required to bring their laptops to the lectures and have a student license of MATLAB®.

Reference Material

Books

- "Numerical Methods for Chemical Engineers with MATLAB® Applications", Constantinides & Mostoufi, Prentice Hall, (2000)
- "Numerical Methods in Engineering with MATLAB®", J. Kiusalaas, Cambridge University Press, (2006)

Online (E-Books available from McGill University Library)

- "MATLAB: A Practical Introduction to Programming and Problem Solving (Second ed.), Attaway, S., Elsevier (2012).
- "Essential MATLAB for Engineers and Scientists", Hahn B. H. & Valentine, D. T., Academic Press (2010).

Instructional Methods

The course will involve lectures, modules and in class problems. *Students are not permitted to record audio or video or take photos of class content!*

Evaluation and Assessment

The students will be responsible for submitting assignments and any in class projects online. A penalty of 10% per day will be issued to all assignments/projects that are submitted past the due date. No marks pertaining to the code and execution of the program will be awarded if the students program does not compile! Assignments and projects must be submitted in report form as a PDF. The computer code must also be submitted, separately, with instructions on how to execute it successfully. All weight of a missed examination will be carried to the remaining exams for the course. *Under no circumstances will there be make up exams!*

Mark Distribution

- Assignments 50%
- Term project 20%
- Exam 1 15% *October 12, 2017*
- Exam 2 15% *November 16, 2017*