The University of Western Ontario
Faculty of Engineering

DEPARTMENT OF CHEMICAL AND BIOCHEMICAL ENGINEERING

CBE 2291b – Computational Methods for Engineers

Course Outline 2014-2015

The objective of this module is to introduce model formulation for various chemical, biochemical and environmental processes, and numerical techniques in solving the associated equations. The module introduces a variety of numerical methods and their application to the solution of problems in the chemical engineering field. These problems include linear and nonlinear algebraic equations, root problems, numerical optimization, finite difference methods, interpolation, linear and nonlinear regression analysis, differentiation and integration, and ordinary differential equations (initial value and boundary value problems). MATLAB will be introduced and extensively used as the computing tool to solve all the above-mentioned problems. Students will learn both the object oriented programming and command line modes of MATLAB and apply them to the solution of a variety of problems involving optimization and dynamic simulation of engineering processes.

Pre-requisites:
Engineering Science 036a/b or Computer Science 026a/b or the former Computer Science 036a/b

Unless you have either the prerequisites for this course or written special permission from your Dean to enroll in it, you may be removed from this course and it will be deleted from your record. This decision may not be appealed. You will receive no adjustment to your fees in the event that you are dropped from a course for failing to have the necessary prerequisites.

Co-requisites: None

Anti-requisites: None

Contact Hours: 3 lecture hours (Tuesdays 10:30-11:30, SEB-3109, and Thursdays 8:30-10:30 SEB-1059), 2 tutorial hours (Wednesdays 9:30-10:30, HCB14/16), 0.5 course.

Instructor(s):

Lars Rehmann (TEB 459) lrehmann@uwo.ca

Undergraduate Assistant: (TEB 477) 519-661-2111 ext: 82131

Course Notes:
Course Notes will be available on the course's OWL site.

Reference Texts: There are many Numerical Analysis books available in the library. Some of them are listed here. Students may make use of any of the following books.

1. Applied Numerical Methods with MATLAB for Engineers and Scientists, 3/e, Steven C. Chapra, McGraw-Hill Higher Education, 2012
2. Applied Numerical Analysis, Curtis F. Gerald and Patrick O. Wheatly, Addison-Wesley, 1999.
3. MATLAB for Engineers, Holly Moore, Pearson Prentice Hall, 2007. ISBN 0-13-187244-3.
4. Numerical Methods: Algorithms and Applications, Laurene V. Fausett, Pearson Prentice Hall, 2003. ISBN 0-13-031400-5.
5. Numerical Methods with MATLAB: Implementation and Application, Gerald Recktenwald,
   Prentice Hall, 2000. ISBN 0-201-30860-6.
6. Problem Solving in Chemical Engineering with Numerical Methods, Michael B. Cutlip and Mordechai Shacham, Prentice-Hall, 1999. ISBN 0-13-862566-2
7. Numerical Methods for Engineers, Steven C. Chapra and Raymond P. Canale, McGraw Hill, 1998.
8. Numerical Methods for Chemical Engineers with Matlab Applications, A. Constantinides and N. Mostoufi, Prentice Hall International, 1999.
9. Numerical Analysis, Timothy Sauer, Addision Wesley, 2006, ISBN 0-321-26898-9.
10. Ajay K. Ray and Santosh K. Gupta, "Mathematical Methods in Chemical and Environmental Engineering", Thomson Learning, 2nd Edition Revised, 2005. ISBN 981-243-935-8.

Laboratory: None

Units: SI and other units will be used.

General Learning Objectives

Knowledge Base	√	Individual Work	√	Ethics and Equity	x
Problem Analysis	√	Team Work	√	Economics and Project Management	x
Investigation	√	Communication	√	Life-Long Learning	√
Design	√	Professionalism	x		
Engineering Tools	√	Impact on Society	x		

Detailed Course outline and Learning objectives

Introduction to numerical software packages

Introduction to Matlab, Scilab, GNU Octave, Freemat and Sage. Course predominately uses Matlab, which will be introduced in detail. Introduction to MATLAB, introducing the theory of variable and matrices, basic operations and plotting**.** Introduction to process modeling and simulation, Examples of chemical, Biochemical and environmental engineering problems arising in fluid mechanics, thermodynamics, heat and mass transfer, separation processes, reaction engineering, process dynamics, and transport phenomena. Introducing advanced visualizations commands in MATLAB. Introduction to basic built-in MATLAB functions. Getting familiar with building user-defined functions, and understanding the importance of them for solving advanced chemical engineering models. Practicing basic flow-control in MATLAB by applying *if, else, elseif, for, while* loops in various problems.

Roots and Optimization

After this section students will:

- Have understanding of what roots problems are and where they occur in engineering and science.
- Know how to determine a root graphically, and though the incremental search method and be aware of shortcomings.
- Know how to solve a roots problem with the bisection method and how to estimate the error of bisection and why it differs from error estimates for other types of root location algorithms.
- Recognize the difference between bracketing and open methods for root location.
- Know how to solve a roots problem with the Newton-Raphson method and appreciating the concept of quadratic convergence.
- Understand why and where optimization occurs in engineering and scientific problem solving and recognize the difference between one-dimensional and multi-dimensional optimization.
- Distinguish between global and local optima.
- Be able to define the golden ratio and understand why it makes one-dimensional optimization efficient.
- Be able to locate the optimum of a single-variable function with the golden-section search, with parabolic interpolation and Matlab's `fminbnd` function.
- Be able to develop MATLAB contours and surface plots to visualize two-dimensional functions.
- Know how to apply the `fminsearch` function to determine the minimum of a multidimensional function.

Linear Algebra

After this section students will:

- Have and understanding matrix notation.
- Be able to identify the following types of matrices: identity, diagonal, symmetric, triangular, and tridiagonal.
- Know how to represent a system of linear equations in matrix form, and how to

solve linear algebraic equations with left division and matrix inversion in MATLAB

- Know how to solve small sets of linear equations with the graphical method and Cramer's rule.
- Understand how to implement forward elimination and back substitution as in Gauss elimination.
- Understand the concepts of singularity and ill-condition.
- Understand how partial pivoting is implemented and how it differs from complete pivoting.
- Recognize how the banded structure of a tridiagonal system can be exploited to obtain extremely efficient solutions.
- Understand that *LU* factorization involves decomposing the coefficient matrix into two triangular matrices that can then be used to efficiently evaluate different right-hand-side vectors, and know how to express Gauss elimination as an *LU* factorization.
- Understand in general terms what happens when MATLAB's backslash operator is used to solve linear systems.
- Know how to determine the matrix inverse in an efficient manner based on *LU* factorization, and how to use the matrix inverse to assess stimulus-response characteristics of engineering systems.
- Understand the meaning of matrix and vector norms and how they are computed, and how to use norms to compute the matrix condition number.
- Understand how the magnitude of the condition number can be used to estimate the precision of solutions of linear algebraic equations.
- Understand the difference between the Gauss-Seidel and Jacobi methods.
- Know how to assess diagonal dominance and knowing what it means.
- Recognize how relaxation can be used to improve convergence of iterative methods.
- Understand how to solve systems of nonlinear equations with successive substitution and Newton-Raphson.

Regression and Interpolation

After this section students will:

- Be familiar with some basic descriptive statistics and the normal distribution.
- Know how to compute the slope and intercept of a best-fit straight line with linear regression.
- Know how to compute and understand the meaning of the coefficient of determination and the standard error of the estimate.
- Understand how to use transformations to linearize nonlinear equations so that they can be fit with linear regression.
- Know how to implement linear regression with MATLAB.
- Know how to implement polynomial regression.
- Know how to implement multiple linear regression.
- Understand the formulation of the general linear least-squares model.

- Understand how the general linear least-squares model can be solved with MATLAB using either the normal equations or left division.
- Understand how to implement nonlinear regression with optimization techniques.
- Recognize that evaluating polynomial coefficients with simultaneous equations is an ill-conditioned problem.
- Know how to evaluate polynomial coefficients and interpolate with MATLAB's polyfit and polyval functions.
- Know how to perform an interpolation with Newton's polynomial and with a Lagrange polynomial.
- Know how to solve an inverse interpolation problem by recasting it as a roots problem.
- Appreciate the dangers of extrapolation by recognizing that higher-order polynomials can manifest large oscillations.
- Understand that splines minimize oscillations by fitting lower-order polynomials to data in a piecewise fashion.
- Recognize why cubic polynomials are preferable to quadratic and higher-order splines.
- Understand the differences between natural, clamped, and not-a-knot end conditions.
- Know how to fit a spline to data with MATLAB's built-in functions.
- Understand how multidimensional interpolation is implemented with MATLAB.

Integration and Differentiation

After this section students will:

- Recognize that Newton-Cotes integration formulas are based on the strategy of replacing a complicated function or tabulated data with a polynomial that is easy to integrate.
- Knowing how to implement the following single application Newton-Cotes formulas: Trapezoidal rule (also as composite formula), Simpson's 1/3 rule, and Simpson's 3/8 rule (also as composite formula).
- Understand how Richardson extrapolation provides a means to create a more accurate integral estimate by combining two less accurate estimates.
- Understand how Gauss quadrature provides superior integral estimates by picking optimal abscissas at which to evaluate the function.
- Know how to use MATLAB's built-in functions `quad` and `quadl` to integrate functions.
- Understand the application of high-accuracy numerical differentiation formulas for equispaced data, and know how to evaluate derivatives for unequally spaced data.
- Understand how Richardson extrapolation is applied for numerical differentiation.
- Recognize the sensitivity of numerical differentiation to data error.
- Know how to evaluate derivatives in MATLAB with the `diff` and `gradient`

functions.
- Know how to generate contour plots and vector fields with MATLAB.

Ordinary Differential Equations
After this section students will:
- Understand the meaning of local and global truncation errors and their relationship to step size for one-step methods for solving ODEs.
- Know how to implement the following Runge-Kutta (RK) methods for a single ODE: Euler, Heun, Midpoint, and Fourth-Order RK
- Know how to iterate the corrector of Heun's method.
- Know how to implement the following Runge-Kutta methods for systems of ODEs: Euler, Fourth-order RK
- Understand how the Runge-Kutta Fehlberg methods use RK methods of different orders to provide error estimates that are used to adjust step size.
- Be familiar with the built-in MATLAB function for solving ODEs.
- Learn how to adjust options for MATLAB's ODE solvers.
- Learn how to pass parameters to MATLAB's ODE solvers.
- Understand what is meant by stiffness and its implications for solving ODEs.
- Understand the difference between initial-value and boundary-value problems.
- Know how to implement the shooting method for linear ODEs by using linear interpolation to generate accurate "shots."
- Understand how derivative boundary conditions are incorporated into the shooting method.
- Know how to solve nonlinear ODEs with the shooting method by using root location to generate accurate "shots."

Evaluation:

The final course mark will be determined as follows:

Assignments 20%
Quizzes 20%
Midterm 20%
Final Examination 40%

Examination will be conducted on a computer and will be **open book**. Only notes and access to OWL are allowed. Use of the internet **for anything other than OWL** is **not** allowed.

Note: Students must pass the final examination to pass this course. Students who fail the final examination will be assigned 48% if the aggregate mark is higher than 50%, or the aggregate mark. **Assignments are to be handed in electronically through OWL on the specified due date provided by the Instructor, unless otherwise directed.**

Use of English:
In accordance with Senate and Faculty Policy, students may be penalized up to 10% of

the marks on all assignments, tests, and examinations for the improper use of English. Additionally, poorly written work with the exception of the final examination may be returned without grading. If resubmission of the work is permitted, it may be graded with marks deducted for poor English and/or late submission.

Attendance

Attendance in all lectures, tutorials and laboratories is mandatory. Any student who, in the opinion of the instructor, is absent too frequently from class or laboratory periods in any course, will be reported to the Dean (after due warning has been given). On the recommendation of the Department concerned, and with the permission of the Dean, the student will be debarred from taking the regular examination in the course.

Cheating

University policy states that cheating is a scholastic offence. The commission of a scholastic offence is attended by academic penalties, which might include expulsion from the program. If you are caught cheating, there will be no second warning (see Scholastic Offence Policy in the Western Academic Calendar).

Plagiarism

Students must write their essays and assignments in their own words. Whenever students take an idea, or a passage from another author, they must acknowledge their debt both by using quotation marks where appropriate and by proper referencing such as footnotes or citations. Plagiarism is a major academic offence (see Scholastic Offence Policy in the Western Academic Calendar).

The University of Western Ontario has software for plagiarism checking. Students may be required to submit their work in electronic form for plagiarism checking.

Conduct:

Students are expected to arrive at lectures on time, and to conduct themselves during class in a professional and respectful manner that is not disruptive to others.

Sickness and Other Problems:

Students should immediately consult with the Undergraduate Services if they have any problems that could affect their performance in the course. Where appropriate, the problems should be documented (see attached). The student should seek advice from Undergraduate Services regarding how best to deal with the problem. Failure to notify Undergraduate Services immediately (or as soon as possible thereafter) will have a negative effect on any appeal.

Notice:

Students are responsible for regularly checking their email and notices posted on the dedicated OWL site.

Consultation:

Students are encouraged to discuss problems with their teaching assistant and/or instructor in tutorial sessions. Office hours will be arranged for the students to see the instructor and teaching assistants. Other individual consultation can be arranged by appointment with the appropriate instructor.

Accreditation (AU) Breakdown

Math	= 50%
Engineering Science	= 30%
Engineering Design	= 20%

January 18, 2014/LR

Western Engineering

The University of Western Ontario
Faculty of Engineering
2014-2015

INSTRUCTIONS FOR STUDENTS UNABLE TO WRITE TESTS OR EXAMINATIONS OR SUBMIT ASSIGNMENTS AS SCHEDULED

IF, ON MEDICAL OR COMPASSIONATE GROUNDS, YOU ARE UNABLE TO WRITE TERM TESTS OR FINAL EXAMINATIONS OR COMPLETE COURSE WORK BY THE DUE DATE, YOU SHOULD FOLLOW THE INSTRUCTIONS LISTED BELOW. YOU SHOULD UNDERSTAND THAT ACADEMIC ACCOMMODATION WILL NOT BE GRANTED AUTOMATICALLY ON REQUEST. YOU MUST DEMONSTRATE TO YOUR DEPARTMENT (OR THE UNDERGRADUATE SERVICES OFFICE IF YOU ARE IN FIRST YEAR) THAT THERE ARE COMPELLING MEDICAL OR COMPASSIONATE GROUNDS THAT CAN BE DOCUMENTED BEFORE ACADEMIC ACCOMMODATION WILL BE CONSIDERED. DIFFERENT REGULATIONS APPLY TO TERM TESTS, FINAL EXAMINATIONS AND LATE ASSIGNMENTS. READ THE INSTRUCTIONS CAREFULLY. (SEE THE 2014 UWO ACADEMIC CALENDAR).

A. *GENERAL REGULATIONS & PROCEDURES*

1. Check the course outline to see if the instructor has a policy for missed tests, examinations, late assignments or attendance.

2. Bring your request for academic accommodation to the attention of the chair of your (or the Undergraduate Services office if you are in first year) PRIOR to the scheduled time of the test or final examination or due date of the assignment. If you are unable to contact the relevant person, leave a message with the appropriate department (or with the Undergraduate Services Office if you are in first year). The address, telephone and fax numbers are given at the end of these instructions. Documentation must be provided as soon as possible.

3. If you decide to write a test or an examination you should be prepared to accept the mark you earn. Rewriting tests or examinations or having the value of a test or examination reweighted on a retroactive basis is not permitted.

B. *TERM TESTS*

1. If you are unable to write a term test, inform your instructor and the Chair of your Department (or the Undergraduate Services Office if you are in first year) PRIOR to the scheduled date of the test. If the instructor is not available, leave a message for him/her at the department office and inform the Chair of the Department (or the Undergraduate Services Office if you are in first year).

2. Be prepared to provide supporting documentation to the Chair and the Undergraduate Services Office (see next page for information on documentation).

3. Discuss with the instructor if and when the test can be rescheduled. **N.B.** The approval of the Chair (or the Undergraduate Services Office if you are in first year) is required when rescheduling term tests.

C. *FINAL EXAMINATIONS*

1. If you are unable to write a final examination, contact the Undergraduate Services Office PRIOR TO THE SCHEDULED EXAMINATION TIME to request permission to write a Special Final Examination. If no one is available in the Undergraduate Services Office, leave a message clearly stating your name & student number (please spell your full name).

2. Be prepared to provide the Undergraduate Services Office with supporting documentation (see next page for information on documentation) the next day, or as soon as possible (in cases where students are hospitalized). The following circumstances are not considered grounds for missing a final examination or requesting special examinations: common cold, sleeping in, misreading timetable and travel arrangements.

3. In order to receive permission to write a special examination, you must obtain the approval of the Chair of the Department **and** the Associate Dean and in order to apply you must sign a "Recommendation for a Special Examination Form" available in the Undergraduate Services Office. The Undergraduate Services Office will then notify the course instructor(s) and reschedule the examination on your behalf.

N.B. **It is the student's responsibility to check the date, time and location of the special examination.**

D. *LATE ASSIGNMENTS*

1. Advise the instructor if you are having problems completing the assignment on time (**prior** to the due date of the assignment).
2. Be prepared to provide documentation if requested by the instructor (see reverse side for information on documentation).
3. If you are granted an extension, establish a due date. The approval of the Chair of your Department (or the Associate Dean if you are in first year) is not required if assignments will be completed prior to the last day of classes.
4. i) Extensions beyond the end of classes must have the consent of the instructor, the department Chair and the Associate Dean. Documentation is mandatory.
   ii) A Recommendation of Incomplete Form must be filled out indicating the work to be completed and the date by which it is due. This form must be signed by the student, the instructor, the department Chair and the Associate Dean.

E. *SHORT ABSENCES*

If you miss a class due to a minor illness or other problems, check your course outlines for information regarding attendance requirements and make sure you are not missing a test or assignment. Cover any readings and arrange to borrow notes from a classmate.

F. *EXTENDED ABSENCES*

If you are absent more than one week or if you get too far behind to catch up, you should consider reducing your workload by dropping one or more courses. (Note drop deadlines listed below). You may want to seek advice from the academic counsellor in your Department or Ms Karen Murray in the Undergraduate Services Office if you are in first year.

G. *DOCUMENTATION*

If you consulted an off-campus doctor or Student Health Services regarding your illness or personal problem, **you must provide the doctor with a Student Medical Certificate** to complete at the time of your visit and then bring it to the Department (or the Undergraduate Services Office if you are in first year). **This note must contain the following information: severity of illness, effect on academic studies and duration of absence.**

In Case of Serious Illness of a Family Member: Provide a Student Medical Certificate to your family member's physician to complete and bring it to the Department (or the Undergraduate Services Office if you are in first year).

In Case of a Death: Obtain a copy of the death certificate or the notice provided by the funeral director's office. You must include your relationship to the deceased and bring it to the Department (or the Undergraduate Services Office if you are in first year).

For Other Extenuating Circumstances: If you are not sure what documentation to provide, ask the Departmental Office (or the Undergraduate Services Office if you are in first year) for direction.

Note: Forged notes and certificates will be dealt with severely. To submit a forged document is a scholastic offence (see below).

H. *ACADEMIC CONCERNS*

You need to know if your instructors have a policy on late penalties, missed tests, etc. This information may be included on the course outlines. If not, ask your instructor(s).

You should also be aware of attendance requirements in some courses. You can be debarred from writing the final examination if your attendance is not satisfactory.

If you are in academic difficulty, check out the minimum requirements for progression in the calendar. If in doubt, see your academic counsellor.

Calendar References: Check these regulations in your 2014 Western Academic Calendar available at www.westerncalendar.uwo.ca.

Absences Due to Illness: http://www.westerncalendar.uwo.ca/2014/pg117.html#
Academic Accommodations for Students with Disabilities: http://www.westerncalendar.uwo.ca/2014/pg118.html
Academic Accommodations for Religious or Holy Days: http://www.westerncalendar.uwo.ca/2014/pg119.html
Course Withdrawals: http://www.westerncalendar.uwo.ca/2014/pg157.html
Examinations: http://www.westerncalendar.uwo.ca/2014/pg129.html
Scheduling of Term Assignments: http://www.westerncalendar.uwo.ca/2014/pg97.html
Scholastic Offences: http://www.westerncalendar.uwo.ca/2014/pg113.html
Student Medical Certificate: http://www.uwo.ca/univsec/pdf/academic_policies/appeals/medicalform.pdf
Engineering Academic Regulations: http://www.westerncalendar.uwo.ca/2014/pg1442.html

Note: These instructions apply to all students registered in the Faculty of Engineering regardless of whether the courses are offered by the Faculty of Engineering or other faculties in the University.

***Drop Deadlines*:**		
	First term half course (i.e. "A" or "F"):	November 5, 2014
	Full courses and full-year half courses (i.e. "E","Y" or no suffix):	November 30, 2014
	Second term half or second term full course (i.e. "B" or "G"):	March 7, 2015

Undergraduate Services Office:	SEB	2097	telephone: (519) 661-2130	fax: (519) 661-3757
Dept. of Chemical and Biochemical Engineering & Green Process Engineering	TEB	477	telephone: (519) 661-2131	fax: (519) 661-3498
Dept. of Civil and Environmental Engineering:	SEB	3005	telephone: (519) 661-2139	fax: (519) 661-3779
Dept. of Electrical and Computer Engineering, Software Engineering, Mechatronics Engineering	TEB	279	telephone: (519) 661-3758	fax: (519) 850-2436
Dept. of Mechanical and Materials Engineering:	SEB	3002	telephone: (519) 661-4412	fax: (519) 661-3020