Mathematical Methods in Chemical Engineering - Syllabus

ChE 2410

Fall 2016

wilmerlab.com/mathmethods.php

Tuesdays, 6:30–8:45PM in room 938 Benedum Hall

Instructor: **Prof. Christopher E. Wilmer**

Office: 903 Benedum Hall

Email: wilmer@pitt.edu

Office hours: To be determined…

Course Description

The objective of this course is to learn mathematical methods used in chemical engineering -- primarily those dealing with solving differential equations. By the end of the course students should be able to apply these methods to tackle the kinds of problems that appear in chemical engineering research.

Course Grades & Policies

The grade earned at the end of the course will be determined by:

Homework	25%
Midterm exam	25%
Final project	25%
Final exam	25%
Total	100%

- **Homework:** There will be four homework assignments, each worth 6.25% of the overall course grade. The assignments will focus on recently covered material, so it is important to attend as many classes as possible to be able to keep up with the homework. Assignments must be handed in at the beginning of class on the day they are due, or if submitted by email (as a PDF file) they must arrive in my inbox before the start of that class. Late homework assignments will receive a 50% penalty if they are handed in before the start of the following class, and 0% after that.
- **Midterm exam:** The midterm exam will be in class. The use of any outside material, such as textbooks or notes, is NOT allowed. Calculators will also not be allowed (they would not help you answer the exam questions anyway).
- **Final exam:** The final exam will be very similar to the midterm exam, except that it will focus on material covered in the second half of the course (but there may still be questions based on material from the first half of the course). The use of any outside material, such as textbooks or notes, is NOT allowed. Calculators will also not be allowed (they would not help you answer the exam questions anyway).

- **Final project:** For the final project, students will work in groups of 2-3 to study a mathematical method NOT covered by the instructor. An approved list of mathematical methods will be provided (see below), and students must declare their choice two weeks prior to the final project's due date: the last day of class. On the last day of class (Dec. 6th) students will give a short presentation on their researched method and submit a three page report. The grading breakdown is given below:

Presentation (5 minutes):		**Report (3 pages, 12pt font, 1" margins):**	
Technical depth	20%	Technical depth	30%
Clarity of presentation	15%	Clarity of writing	10%
Stays within time limits	15%	Proper citation use	10%

Technical depth: Did demonstrate an understanding of the method? Did you explain how the method was derived or how to apply it to a difficult problem?

Clarity of presentation: Did you clearly explain the method? Did you speak loudly? Were your diagrams and equations large enough so that people at the back of the room could easily see them? Did you practice your presentation in front of someone before presenting it in class?

Stays within time limits: To get a perfect score on this category, presentations must end within the 5 minute limit. To get 10% (out of 15%) presentations must be under 6 minutes. Presentations over 6 minutes will receive 0% for this category and, to make sure enough time is available for others, the presenters will be asked to immediately stop.

Clarity of writing: Did you clearly explain the method? Do you explain the meaning of technical jargon before using it? Does the report have spelling and/or grammar errors? Did you ask someone to proofread your report before handing it in?

Proper citation use: Did you cite scholarly work (books or journal articles, not encyclopedia articles or online tutorials) where appropriate? Are citations properly formatted (in this class we will use the citation formatting style used by the journal *Nature*)?

List of mathematical methods for the final project:

Finite elements	Machine learning
Spectral methods	Vector calculus
Nonlinear differential equations	Linear algebra
Optimization methods	Monte Carlo method
Conjugate gradient method	Graph/network theory
Fourier analysis	Green's functions
Asymptotic analysis	Complex analysis

Note that these are very broad topics, you are expected pick a narrower subtopic for your project on your own. Once you have picked your topic (& subtopic) you must get it approved by the instructor two weeks prior to the submission deadline. If there is a topic you would like to study that isn't listed, please discuss it with me as soon as possible.

Grading Errors

Sometimes you may receive a grade on a homework assignment or exam that is in error, either due to a simple arithmetic error on the grader's part or because your answer was falsely interpreted to be incorrect. Don't panic. It is very important to bring these to my attention as soon as possible, and provided that you can demonstrate clearly the error on the grader's part, you will receive full credit for your answer. In order to get credit for an incorrectly graded answer, you must send me an email detailing the problem and schedule an appointment in my office. Please refrain from discussing grading errors in class as that time is limited and needed for other purposes.

Missed Exams

Missed exams can be made up under certain, very limited, circumstances, e.g., illness requiring medical care, death in family, or travel related to University or work activities (for part-time students). Requests for make-up exams must consist of 1) an email explaining the reason for missing the exam, and 2) relevant corroborating documentation (e.g., a doctor's note). If you know you will miss an exam, arrangements must be made at least one week in advance of the exam. If the missed exam is unanticipated, the email requesting a make-up exam must be sent no later than one week after the exam. If these rules are not followed for a missed exam, a 0% grade may result.

Academic Integrity

All homework and exams will be completed individually. Consultation with other students is permitted on homework, but not during exams. Violations of the University Academic Integrity Guidelines will result in penalties consistent with those guidelines, which may include receiving a failing grade in the course.

Disability Concerns

If you have a disability for which you are or may be requestion accommodation, you are encouraged to contact both the instructor and Disability Resources and Services (DRS) as early as possible in the semester. DRS is located at 216 William Pitt Union and can be contacted at (412) 648-7890 / (412) 383-7355 (TTY). DRS will verify your disability and determine reasonable accommodations for this course.

Course Outline & Schedule

From a birds-eye view the topics covered in this course are as follows (in order):

Numerical methods
↓
Ordinary differential equations
↓
Partial differential equations

Note: It is not common to begin with numerical methods in a course like this, but given the prominence of computers in research, and the flexibility of numerical methods to a broad range of research problems, I decided it would benefit students the most to emphasize this part.

Below is a breakdown of the topics that we will follow in approximately chronological order. Since a good class is responsive to the needs and interests of its students, we may not follow these subtopics in the exact order listed, and it's possible a subtopic will be skipped and another one added.

0. **Classifying differential equations**
1. **Numerical methods**
    a. Using open-source Jupyter notebooks for mathematical programming
    b. Finite differences & difference operators
    c. Sources of error in finite difference schemes
    d. Explicit vs. implicit schemes
        i. (Explicit) Forward/backward Euler
        ii. (Explicit) Central differencing
        iii. (Explicit) Runge-Kutta method
        iv. (Implicit) Crank-Nicolson
    e. Boundary conditions for the heat equation
2. **Ordinary differential equations (ODEs)**
    a. 1st order: Integrating factor
    b. Nth order (special case): Constant coefficient equations
    c. 2nd order: Homogeneous vs. inhomogeneous equations
    d. 2nd order: Variation of parameters
    e. 2nd order: Power serious solutions & Frobenius theory
    f. 2nd order: Initial value & boundary value problems
    g. 2nd order: Bessel functions
    h. 2nd order: Sturm-Liouville eigenvalue problems
3. **Partial differential equations (PDEs)**
    a. Laplace and Poisson equations
    b. Parabolic, elliptic, and hyperbolic equations
    c. PDEs in three dimensions: parallelepipeds & spheres