CM4450 – Computational Methods in Chemical Engineering

Instructor: Jason Keith
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Office: 202-D Chemical Sciences Building

Course Meeting Times: MW 12:05 – 12:55 MEEM Room 120 (Computer Fishbowl)
Office Hours: TBA, based upon student availability

Reference Texts (placed on reserve in Van Pelt Library under CM4450):

- *Numerical Methods for Engineers*, Steven C. Chapra and Raymond P. Canale (McGraw-Hill)

General description of topics to be covered:

- Part 1: Basics of Numerical Methods
  - Interpolation (week 2)
  - Numerical Differentiation (week 3)
  - Numerical Integration (week 4-5)
- Part 2: Numerical Solution of Ordinary Differential Equations (weeks 6-10)
- Part 3: Numerical Solution of Partial Differential Equations (weeks 10-13)
- Part 4: Using COMSOL Multiphysics (week 14)

Course Format: This class will meet twice a week (Mondays and Wednesdays). Each class will start with lecture covering theory and applications of the topic to be discussed. There will be breaks to solve in-class problems with and without the classroom computers. Students will also be able to use class time to work individually or in teams on the homework assignments, and ask the instructor for assistance.

Course Goals: Upon completion of this course, you should be able to:

- Use MATLAB to graph and analyze data
- Explain to a student not in this course how to interpolate between data points using simple (linear, quadratic) or advanced (cubic splines) interpolation
- Calculate first and second derivatives of data using simple and advanced (higher order) numerical differentiation techniques
- Integrate numerical data with basic and advanced numerical integration techniques
- Describe the accuracy regarding the interpolation, differentiation, and integration of data
- Solve single and multiple ordinary differential equations using a variety of numerical techniques
- Solve hyperbolic, parabolic, and elliptic partial differential equations using numerical techniques
- Learn how to use Comsol Multiphysics software

Evaluation Tools:

Item	*Weight*
Homework (one or two problems per week)	50 %
Quiz 1 (week 6)	25 %
Quiz 2 (week 13)	25 %

Grading Scale:

Letter Grade	*Percent Range*
A	100.0-90.0%
AB	89.9-80.0%
B	79.9-70.0%
BC	69.9-60.0%
C	59.9-50.0%
CD	49.9-40.0%
D	39.9-30.0%
F	< 30.0%

Instructor's Expectations of the Student: This is an elective course and meant to encourage students to pursue lifelong learning on non-traditional topics. The course will be taught in a problem-based learning format. The instructor will lecture for about half of the class and then the students will work on problems individually or in small teams. Some of these problems will be the "homework" to be turned in later.

Homework policy: Please turn in your homework the day it is due. If it is late you will lose 10% of the possible points for each day it is late unless you make arrangements in advance.

Please write your homework solutions neatly and clearly on engineering problem paper (sold in the bookstore) starting each new problem on a new piece of paper. Please attach the problem statement to your completed homework. Your answers must be placed in a rectangular box (not circled). You will lose points for lack of neatness and clarity. Pretend you're working for a company and **take pride in your work**. Please see the sample problem for an illustrative example. Neatness and clarity will be part of your homework grade.

Please contact me immediately if you feel you deserve more points on your homework. Grade changes on homework assignments must be made within one week of your receipt of the graded homework (that's when we inscribe grades onto stone tablets).

You may work in *study groups* on the homework assignment. Please list the team members you worked with on the homework assignment when you turn it in.

Additional Information:

Course Description: Computational methods for solution of chemical engineering problems in transport phenomena, reaction kinetics, and dynamical systems. Topics include general numerical methods and solution to ordinary and partial differential equations. Advanced use of MATLAB and Comsol Multiphysics software.

University Policies:

Academic regulations and procedures are governed by University policy. Academic dishonesty cases will be handled in accordance the University's policies.

If you have a disability that could affect your performance in this class or that requires an accommodation under the Americans with Disabilities Act, please see me as soon as possible so that we can make appropriate arrangements. The Affirmative Action Office has asked that you be made aware of the following:

Michigan Tech complies with all federal and state laws and regulations regarding discrimination, including the Americans with Disabilities Act of 1990. If you have a disability and need a reasonable accommodation for equal access to education or services at Michigan Tech, please call the Dean of Students Office, at 487-2212. For other concerns about discrimination, you may contact your advisor, department head or the Affirmative Action Office, at 487-3310

Academic Integrity:
http://www.studentaffairs.mtu.edu/dean/judicial/policies/academic_integrity.html

Affirmative Action:
http://www.admin.mtu.edu/aao/

Disability Services:
http://www.admin.mtu.edu/urel/studenthandbook/student_services.html#disability

Equal Opportunity Statement:
http://www.admin.mtu.edu/admin/boc/policy/ch3/ch3p7.htm