University of Minnesota

Department of Chemical Engineering and Materials Science

MATS3141: Numerical Methods for Material Science (3 credits)

Spring Semester 20XX Syllabus

Course Description

There are a very limited number of important problems in Materials Science that can be completely solved analytically. In this class, students learn how to solve problems that are impossible to solve analytically, but are amenable to numerical solution. To achieve this, students will learn how to set up problems and program them using MatLab, make reasonable numerical approximations, and solve these problems numerically and/or graphically. In all cases the problems discussed will be closely focused on Materials Science examples encountered in other junior and senior year classes. Specific important Materials Science examples that will be covered include:

- Oxidation and corrosion problems coupling diffusion and kinetics
- Nucleation and growth problems such as dendritic growth and crystallization
- Solutions to the Schrodinger equation relevant to semiconductor devices
- Solutions to the equations governing electrostatics relevant to electronic devices
- Diffusion problems relevant to processing and synthesis of materials and devices

To enable a proper numerical analysis of these various problems, a review and extension of some major math concepts is also given at the beginning of the class. This will focus in particular on differential equations of the form commonly encountered in Materials Science, as well as Fourier methods. Note that the class is designed to be taken concurrently with MATS3002, Mass Transport and Kinetics, and a large number of the examples and problems will focus on such topics. The classes will nevertheless be available to be taken separately.

The course is organized around the following themes:

Course Objectives

Students enrolled in this course will:

- be given a review and extension of critical mathematical concepts and methods
- be given an introduction to basic numerical methods
- be given an introduction to programming using MatLab
- learn how numerical methods can be applied to solve practical Materials Science problems
- develop an understanding of the potential and limitations of numerical methods in Materials Science and Engineering.

Prerequisites

Math 2373, Linear Algebra and Differential Equations
Math 2374, Multivariable Calculus
Chem 4502, Quantum Mechanics **OR** Phys 2303, Physics III

Books

Required:

"*Numerical Methods with Applications in Chemical Engineering*" by K. Dorfman and P. Daoutidis (currently in press).
"*Mathematical Physics*" by B. Kusse and E.A. Westwig

Optional:

- Stormy Attaway, *MatLab: A Practical Introduction to Programming and Problem Solving*
- Stephen J. Chapman, *MatLab: Programming for Engineers*.
- Brian H. Hahn and Daniel T. Valentine, *Essential MatLab for Engineers and Scientists*

Course Web Site

http://www.moodle.umn.edu/…
The course web site will have links to the lecture notes, homework and exam solutions, practice exams and solutions, and other useful educational links. Do not give the solutions to anyone else; the material is for your own use only. Acting to the contrary will be considered unauthorized collaboration.

Main Instructor

Prof. K. Andre Mkhoyan
Office : 34 Amundson Hall
Phone : (612) 625-2059
Email : mkhoyan@umn.edu
Office Hrs.: M 4:00-5:00 pm and F 4:00-5:00 pm, or by appointment.

Recitation Instructor (TBD)

Prof.
Office :
Phone :
Email :
Office Hrs.:

Teaching Assistants (TAs) (TBD)

Ms./Mr.
Office :
Phone :
Email :
Office Hrs:

Lectures

MWF (~60-70 students anticipated). This will be a required class for Materials Science and Engineering (MSE) majors.

Recitations (solving example problems)

Th (~30-35 students per section)
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The recitations will focus on example problem solving and will involve work in small groups. There will be no formal lecture.

Homework, Exams and Grading Policy

1. The basis of grading will be as follows:

Homework		10%
Exam 1	(Wednesday, Feb. XXth)	25%
Exam 2	(Wednesday, Apr. XXth)	25%
Final	(XXX, May XXth)	40%

   Your letter grade will be determined using your overall score, S, in homework and exams. Your overall score will be determined using:

$$S = \{0.1 \times HW_{avg}\} + \left\{ \sum_{i=1}^{2} (0.25 \times E_i) \right\} + \{0.4 \times E_{final}\},$$

   where,

   HW_{avg} = average of all homework scores
   E_i = exam score for exam i
   E_{final} = final exam score

2. Homework will be posted on the course web site on **Wednesday** after class before midnight and will be due on **Wednesday** at the **beginning of the lecture**. NO EXCEPTIONS. In the case of properly documented family emergencies or illness, the missed homework assignment will not be used in evaluating the student's average homework grade. Homework solutions will be posted on the web site within 24 hours after students have turned in the homework. Students are encouraged to discuss the material and study together in the interest of learning. However, each student is expected to complete their problem sets independently. Students may work on problems together if in the interest of learning. However, problem set solutions must be submitted in the student's own handwriting and reflect the student's own reasoning, words and calculations. Remember that your success in the exams will depend on how well you understand the material and the individual effort you put in the problem sets.
3. Questions and complaints regarding homework or exam grading should be directed to Professor Mkhoyan within a week after the graded work is returned to you. If you ask for a re-grade we will re-grade all parts of the homework and exam in question.

4. The examination and homework due dates are firm. Make up final exams are possible in the case of properly documented family emergencies or illness. Make up final exams will be given after the regularly scheduled exam and will be different than that given in class. While every effort will be made to make exams that are of equal "fairness" and difficulty, students requesting a make up exam acknowledge that they are taking a different exam and agree not to question its difficulty as compared to the in-class exam.
5. There will not be make up midterms. In the case of properly documented family emergencies or illness the missed exam will not be used in evaluating the student's grade; missed exams will be equally distributed between the remaining exams and the Final.
6. Exams are closed book. You may bring an ordinary scientific calculator to the exams.
7. When answering homework and exam questions write neatly and use complete and clear sentences that are your own. Show all your work with a reasonable number of logical steps that leads to the final answer. Numerical answers must have units unless the value is dimensionless. Write your name and last name on the upper right hand corner of your homework and staple all pages together. Please use graph paper or software to produce all graphs in the homework. Label all axis and give units. The instructors and TAs may give no credit when units are omitted from the graphs or numerical answers.

E-mail Policy

In compliance with FERPA and the Minnesota Privacy Act, Students must use their U of M e-mail account for conducting official business with the University of Minnesota. Messages originating from other e-mail accounts will be disregarded.

Student Academic Integrity and Scholastic Dishonesty

"Academic integrity is essential to a positive teaching and learning environment. All students enrolled in University courses are expected to complete coursework responsibilities with fairness and honesty. Failure to do so by seeking unfair advantage over others or misrepresenting someone else's work as your own, can result in disciplinary action. The University Student Conduct Code defines scholastic dishonesty as follows:

> **Scholastic Dishonesty:** Scholastic dishonesty means plagiarizing; cheating on assignments or examinations; engaging in unauthorized collaboration on academic work; taking, acquiring, or using test materials without faculty permission; submitting false or incomplete records of academic achievement; acting alone or in cooperation with another to falsify records or to obtain dishonestly grades, honors, awards, or professional endorsement; altering forging, or misusing a University academic record; or fabricating or falsifying data, research procedures, or data analysis.

Within this course, a student responsible for scholastic dishonesty can be assigned a penalty up to and including an "F" or "N" for the course. If you have any questions regarding the expectations for a specific assignment or exam, ask."

Copying homework solution from others, from solutions to problems posted during previous years and from instructor solution manuals is considered a breach of the above honesty code. Students who breach this code will be reported to the appropriate University authorities, will be given zero on all the homework assignments and may be assigned an "F" in the class.

Software Usage

The primary application used in the class will be MatLab, which students have access to via the UofM / CSE site license. You will be provided with details of how to access this application.

Outline/Schedule

Week	Topic	Assignment
1	Mathematical Models	HW #1
2	Review of Mathematics: Linear Algebra; Review of Mathematics: Norms and Conditioning	HW #2
3	Review of Mathematics: Ordinary Differential Equations (ODEs), Partial Differential Equations (PDEs), with applications in MSE	HW #3
4	Fourier Series, Fourier Transforms, with applications in MSE	HW #4
5	Computer Math/Elements of Computer Algorithms; Elements of Computer Algorithms	HW #5
6	Gauss Elimination, Pivoting and Banded Matrices, Iterative Methods	MidTerm #1
7	Newton's Method, Newton-Raphson Method, Examples of Materials Science problems	HW #6
8	Linear Interpolation, Gauss Quadrature, Examples of Materials Science problems	HW #7
9	Explicit and Implicit Euler Methods, Examples of Materials Science problems	HW #8
10	Higher Order Methods, Systems of ODEs and Higher-Order ODEs, Examples of Materials Science problems	HW #9
11	Finite-Difference Method, Examples of Materials Science problems	HW #10
12	Boundary Value Problems (BVPs), Examples of Materials Science problems	MidTerm #2
13	Method of Lines, Examples of Materials Science problems	HW #11
14	Two-dimensional PDEs, Examples of Materials Science problems	HW #12
15	Numerical Fast Fourier Transforms, Examples of Materials Science problems	