COURSE: COMS 6500 (4 credits): Fundamentals of Scientific Computing

Meeting Times: MW 6:00 p.m. - 7:25 p.m.
Tuesday: One hour Computer Lab: T 6:00-6:55 p.m.

Location: MW: KOM 158, Tuesday: KOM 267

TEXT BOOKS:


Related books and Journal(s):

1. Scientific Computing with Case Studies, by Dianne P. O' Leary

2. Scientific computing with MATLAB, by Par Alfio Quarteroni and Fausto Saleri
   ISBN: 3-540-44362-0, Springer-Verlag, New York

   ISBN 978-3-642-19494-8

4. Numerical Mathematics and Computing, by Ward Cheney, and David Kincaid,


6. SIAM Journal on Scientific Computing

INSTRUCTOR: Dr. A. Q. M. Khaliq, KOM-250, Phone: 615-494-8889
           E-Mail: akhaliq@mtsu.edu

OFFICE HOURS: 1:30-3:00 P.M. M W, and any other time by appointment.
OBJECTIVES:

The course will provide fundamentals of problem solving approach in computational science by learning computer arithmetic and error analysis, linear and nonlinear equations, least squares, interpolation, numerical differentiation and integration, optimization, random number generators and Monte Carlo simulation. Students will gain computational experience by working on case-studies using modern software packages such as MATLAB and advance features of FORTRAN. Computational Science problems from different disciplines will solved as mini case studies.

By the end of the course, a successful student should be able to: understand and apply scientific computing approach for the solution of physical and mathematical problems in Computational Science. Use MATLAB to write clear and structured scripts and functions to implement algorithms.

OUTLINE OF COURSE TOPICS:

- **MATLAB-weekly one hour in Computer Lab**
  Lectures will be given on basic to advanced features of MATLAB. You are responsible to learn most of it by yourself.
  Computational assignments involving case studies are integral part of the course.
  - **Errors and Computer Arithmetic**
    Approximation in scientific computing, Error in computation, computational complexities, floating point arithmetic, ill-conditioning and stability
    Mini Case Study: Avoiding Catastrophic Cancellation
  - **System of Linear Equations**
    Direct and Iterative methods for linear systems, Sensitivity and conditioning,
    Mini Case Study: Solving linear systems using MATLAB.
  - **Nonlinear Equations**
    Solving nonlinear equations using fixed point iteration, Convergence rates,
    Stopping criteria
    Mini Case Study: Solving system of nonlinear equations with MATLAB
  - **Interpolation**
    Polynomial interpolation, Cubic Splines, Radial Bases functions (RBFs)
    Mini Case Study: using MATLAB and other software
  - **Numerical Integration and Differentiation**
    Integration, numerical differentiation
    Computational Assignments: Using MATLAB and other software
  - **Eigenvalue Problems**
    Computing eigenvalues and eigenvectors, matrix and vector norms, Ill-conditioning
  - **Initial Value Problems for ODEs**
    Explicit and Implicit methods for ODEs, Stability and Convergence analyses, Stiff and Non-stiff ODEs.
    Mini Case Study: Use of ODE methods available in MATLAB
• **Random Numbers and Stochastic Simulation**
Randomness and Random numbers, stochastic simulation, Random number generator, Mini Case Study: MATLAB and other software for generating random numbers, and Monte Carlo simulation. Mini Case Study: Monte Carlo simulation

• **Optimization and Data Fitting**
Unconstrained optimization, constrained optimization, Mini Case Study: Use of software for optimization.

**GRADING SCALE:** 90- 100% A; 80-89% B; 70 - 79% C; 60 - 69% D; 00 - 59% F

Grades will be calculated based on the following instruments:

<table>
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<tr>
<th>Instrument</th>
<th>Percentage</th>
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<tbody>
<tr>
<td>Tests</td>
<td>40%</td>
</tr>
<tr>
<td>Computational Assignments &amp; Case Studies</td>
<td>25%</td>
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<tr>
<td>Research Project</td>
<td>15%</td>
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<tr>
<td>Final Exam</td>
<td>20%</td>
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**2 Tests**

(October 12, November 16)

You will be given 2 (2 hours each) tests during the semester. These will be in class tests; each test will carry equal weight, and will cover all the material learned up to and including one day before the exam. Please turn all cell-phones off during the test.

**Computational Assignments and Case Studies:**

You will be given no more than 10-15 computational assignments during the semester. These assignments will include case-studies from different areas of Computational Science. Case studies will involve challenging computational problems. You should strive to start the computational assignment the day it is assigned. Be detailed in your explanations when documenting computational results. Cheating is not tolerated, and will be dealt according to MTSU policy.

**Research Project:**

You will be required to work on a research project related to the course with application to an area in Computational Science. The project will be presented in class, and a short write up will also be required for the grade.

**Final Exam:**

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<th>Date</th>
<th>Time</th>
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<tr>
<td>Monday, December 12</td>
<td>6:00 - 8:00 p.m.</td>
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Final exam will be comprehensive and will be only given according to MTSU Final exam schedule on the above date and time. Please turn all cell-phones off during the Final Exam.
**Homework:**

You will be assigned textbook problems on each day class is held (except for exam days). You should strive to solve the problems the day they are assigned. It is very important to keep up with the homework and do the problems regularly. Some homework problems will be graded, it is very important to do the all the assigned problems for the mastery of the subject.

I encourage you to work with others on homework problems. However, be sure that you understand everything and do not become dependent on others. While I will solve homework problems in class, you may feel free to stop by my office to discuss the problems. Feel free to e-mail me questions you are not able to solve, and I’ll address solutions to such problems in the next lecture.

**Attendance and Late Work Policy:**

Perfect attendance is expected to succeed in the course. To obtain an excused absence due to illness for a day that class meets, you must submit written verification obtained from a physician, or the Office of Student affairs. If you have an excused absence for the day an exam is scheduled, you must contact me to make arrangements for taking a make-up test (which will be different from and perhaps slightly more difficult than the original exam). The make-up Test should be taken as soon as possible, and definitely no later than five days after the original test was administered. Missing a test may mean that you will lose the privilege of obtaining written solutions from me.

If you have an excused absence for the day Assignment is due, you must submit the assignment to me within 48 hours of the time it was due. If you are still on excused absence, you must send someone to bring the assignment to my office before the 48 hours has expired. This deadline is strict so that I may give solutions soon after the assignment is due.

Tests and assignments missed without an excused absence will be recorded as zero points. There will be no other chances to complete missing work, so please keep on top of things.

**IMPORTANT INFORMATION:**

- A grade of “I” will be given only in accordance with university policy.

**DISABILITY STATEMENT:**

If you have a disability that may require assistance or accommodation, or you have questions related to any accommodations for testing, note takers, readers, etc., please speak with me as soon as possible. Students may also contact the Office of Disabled Students Services (898-2783) with questions about such services.

**NOTE:** Syllabus subject to change with notice