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; time to be arranged

Location: Main Campus, Kirksey Old Main Building, KOM 205

TEXT BOOKS:


Other useful book(s):

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

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

OFFICE HOURS: 1:30-3:00 P.M. MTW, 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.

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**
Basic to advanced features of MATLAB will be studied from the recommended text. Notes will be provided for the topics not covered in the text.

- **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 and Stopping criteria.
  Mini Case Study: Solving system of nonlinear equations with MATLAB

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

- **Interpolation**
  Polynomial interpolation, Interpolation using cubic splines.
  Mini Case Study: Using MATLAB for spline interpolation

- **Numerical Integration and Differentiation**
  Integration, numerical differentiation
  Mini Case Study: Using MATLAB and other software

- **Random Numbers and 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.

- **Case Studies and Projects**
  Projects from different disciplines in Computational Science

**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:

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<thead>
<tr>
<th>Instrument</th>
<th>Percentage</th>
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<tr>
<td>Tests</td>
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<td>Assignments</td>
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<td>&amp; Case Studies</td>
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<td>Project</td>
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<td>Final Exam</td>
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2 Tests

(October 06, November 10)

You will be given 2 tests during the semester. These will be in class closed-book tests; Each test will carry equal weight, and will cover all of 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 computational assignments during the semester. These assignments will also 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 to be 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:

| Monday, December 13 | 6:00 - 8:00 p.m. |

Final exam will be comprehensive, closed book exam 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. Although home work problems will not be graded, it is very important to do the 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