EECE 7220/8220: Scientific Computing (Syllabus)

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EECE 7220 / 8220
Scientific Computing
Spring Semester 2024

Regular Lectures: ES 220; Monday and Wednesday, 12.40 pm to 2.05 pm

Instructor: Madhu Balasubramanian
Office: 208D Engineering Science Building
Telephone: (901) 678-1199
Email: mblsbrmn@memphis.edu (more reliable)
Office hours: By appointment (flexible; email for appointment)

Recommended Text
a. Lecture notes

Additional References
   Electronic copy: https://www-users.cs.umn.edu/~saad/IterMethBook_2ndEd.pdf

Website: https://memphis.instructure.com/

Prerequisites: Graduate standing or consent of the instructor

Grades
- Attendance
- Homework and programming assignments
- Letter grade assignment (may change to match class average)
  A+: 98 to 100;  A: 92.5 to 97.9;  A-: 90.0 to 92.4
  B+: 87.5 to 89.9;  B: 82.5 to 87.4;  B-: 80.0 to 82.4
  C+: 77.5 to 79.9;  C: 72.5 to 77.4;  C-: 70.0 to 72.4
  D+: 67.5 to 69.9;  D: 62.5 to 67.4;  D-: 60.0 to 62.4
  F: 0.0 to 59.5

Course Objectives:
- Prepare for scientific computing work at the graduate level.
- Learn well-established scientific computing techniques
- Lay foundation for advanced computing work in various areas of research.
d. Incoming graduate students will benefit from the review of mathematical preliminaries and programming experience through homework.

University Guidelines for Covid-19:
https://www.memphis.edu/coronavirusupdates/

Important Dates:
https://www.memphis.edu/registrar/calendars/academic/ay2324.php
- M. L. King, Jr. Holiday: January 15, 2024 / Monday
- First Day of Classes: January 16, 2024 / Tuesday
- Spring Break: March 4-10, 2024 / Monday-Sunday
- Last Day of Classes: April 24, 2024 / Wednesday
- Study Day: April 25, 2024 / Thursday
- Exams: April 26 - May 2, 2024 / Friday-Thursday

https://www.memphis.edu/registrar/calendars/exams/24s-final-exams.php
- Final Exam: Wednesday, May 1, 2024, 10 am to 12 noon

My Teaching Philosophy:
- I believe that motivation in a course is an important factor in learning. A significant part of the initial motivation in a topic often comes from gaining a comprehensive view of the subject as well as its uses. Further, it is essential to preserve or further enhance the initial motivation when complex topics are introduced as the course progresses. I will remind the class how each of my lectures fit into the course, the overall subject matter and when applicable, how the lecture is relevant to areas that the students are majoring in and in their professional career.
- I will review relevant and necessary background materials (e.g. linear algebra concepts) that may engage the learners and encourage them to further strengthen their foundational knowledge through self and assisted learning. Further, it may lay a coherent and stronger foundation for learning newer and advanced concepts.
- I encourage students to develop perseverance to learn and master newer concepts i.e. keep practicing and don’t give up.

Class Participation:
- I expect the students to fully engage in the learning activities, group activities and participate in class discussion.
- Students should feel at ease to seek clarification at any stage in this course during lecture, and after lecture through individual appointment (seek appointment by email).

I encourage students to utilize the class discussion forum setup in Canvas to seek additional clarification regarding lectures and course materials, share your thoughts on
questions from other students in class. While using the group discussion forum, please following the following etiquette:

- Please use the discussion tool to seek clarification.
- Feel free to participate in discussion, and answer questions.
- Be respectful to others during discussion.
- For each topical question, open a new thread
- Answer any questions by responding to the question within the thread.

Academic Integrity:

Plagiarism, cheating and other forms of academic dishonesty are prohibited. Students guilty of academic misconduct, either directly or indirectly, through participation or assistance, are immediately responsible to the instructor of the class in addition to other possible disciplinary sanctions which may be imposed through the regular institutional disciplinary procedures. Expectations for academic integrity and student conduct are described in detail on the website of the Office of Student Accountability. Please read in particular, the section about "Academic Misconduct". Also refer to https://www.memphis.edu/osa/pdfs/csrr.pdf

Resources:

- **Canvas** (learning management system) will be used to distribute lecture materials (slides, videos, notes), quizzes, and homework problems; submit assignments, and exam solutions; and for offline discussion including for seeking clarification and sharing your thoughts: https://www.memphis.edu/um3d/canvas/index.php

- Learning to use Canvas: https://www.memphis.edu/um3d/canvas/index.php

- Citrix has a comprehensive collection of engineering software such as Matlab and commonly used software such as Photoshop. You can access Citrix online with the following URL: https://citrix.memphis.edu/vpn/index.html

Syllabus Changes

The instructor reserves the right to make changes as necessary to this syllabus. If changes are necessitated during the term of the course, the instructor will immediately notify students of such changes both in class and in eCourseware.

Students with Disabilities

Qualified students with disabilities will be provided reasonable and necessary academic accommodations if determined eligible by disability services staff at the University of Memphis. Prior to granting disability accommodations in this course, the instructor must receive written verification of a student's eligibility for specific accommodations from the disability services staff. It is the student's responsibility to initiate contact with Disability Resources for Students (DRS) and to follow the established procedures for having the accommodation notice sent to the instructor.

Sexual Misconduct and Domestic Violence Policy

This policy specifically addresses sexual misconduct which includes dating violence, domestic violence, sexual assault, and stalking. The policy establishes procedures for
responding to Title IX-related allegations of sexual misconduct. Complaints can be reported to the Office for Institutional Equity (OIE). You may contact OIE by phone at 901.678.2713 or by email at oie@memphis.edu. Complaints can be submitted online at File a Complaint. OIE’s office is located at 156 Administration Building.

**Non-Discrimination and Anti-Harassment Policy**

University policy prohibiting discrimination and harassment based on protected characteristics and classes. Complaints of discrimination and harassment can be reported to the Office for Institutional Equity (OIE). You may contact OIE by phone at 901.678.2713 or by email at oie@memphis.edu. The full text of the policy can be found at [GE2030 - Non-Discrimination and Antiharassment](#).
Catalog Title Abbreviation: Scientific Computing

Catalog Description: Review of scientific computing mathematical preliminaries. Topics include numerical linear algebra, orthogonality, eigenvalues, boundary value problems, integral equations and Green's functions, numerical integration, basic iterative methods, preconditioning, parallel programming, and advanced topics.

Course Outline:

a. Motivation: $Ax = b$, solving for $x$
   i. $A$: system matrix
   ii. Discretizing and solving partial differential equations governing any system (e.g. finite element method, finite volume method, finite difference method)
   iii. A deep learning model as a composition of piecewise linear functions and non-linear (activation) functions: $F(W, v) = L_2\left(W_2, N_1\left(L_1(W_1, v)\right)\right)$, where, $L(W, v) = Wv + b$

b. Numerical linear algebra
   i. Brief review of linear algebra
   ii. Terms and definitions
   iii. Types of matrices
   iv. Definition of a vector space
   v. Linear independence of functions, subspace, basis and dimension
   vi. Innerproduct, norm and their properties
   vii. Range (column space), null space and rank of a matrix
   viii. Eigensystems and spectrum of a matrix
   ix. Condition number of a matrix
   x. Matrix inverse
   xi. Orthogonality, orthogonal matrix and unitary matrix
   xii. Normal matrix
   xiii. Matrix decompositions: Cholesky ($A = LL^T$), Schur ($A = QTQ^*$), SVD ($A = U\Sigma V^*$)
   and Spectral decomposition ($A = V\Lambda V^{-1}$)
xiv. Definiteness: positive and negative definiteness, semi-definiteness, symmetric positive definiteness and Hermitian

c. Orthogonality, and orthogonalization procedures
   i. Gram-Schmidt orthogonalization procedure
   ii. Householder transformation

d. Introduction to parallel programming and message passing interface (MPI)

e. Eigenvalues and Eigenvectors
   i. Computing the eigenvalues and eigenvectors
   ii. Example problems: 1) solving a system of differential equations, 2) quantum mechanics, 3) Fibonacci series, 4) Markov process

f. Condition number, floating point arithmetic (round off errors) and stability

g. Conditioning and stability of least squares algorithms

h. Direct methods for solving $Ax = b$
   i. Iterative solution to linear algebraic system of equations
i. Projection operators: orthogonal and oblique

ii. Orthogonal projection operators

iii. Solution by imposing the Petrov-Galerkin condition

iv. Steepest descent (special, residual normal steepest descent)

j. Basic iterative methods:
   i. Jacobi iterative method,
   ii. Gauss-Seidel method
   iii. Successive over-relaxation method
   iv. Convergence properties

k. Subspace methods on Krylov subspaces:
   i. Krylov subspaces
   ii. Arnoldi's method
   iii. Generalized minimal residual method
   iv. Conjugate gradient method
   v. Conjugate residual method
   vi. Bi-conjugate gradient method

l. Preconditioning techniques for iterative methods

m. Multiresolution / Multigrid techniques

n. Domain decomposition methods (in the context of preconditioning to iterative methods and parallel computing)

o. Unconstrained optimization problems
   i. Learning from data / machine learning
   ii. Loss function, Taylor expansion
   iii. Newton's method
   iv. Gradient descent vs steepest descent vs conjugate gradient
   v. Stochastic gradient descent
   vi. Learning network weights in deep learning using backpropagation (BP – compute derivatives using chain rule in a computational graph)

p. Solving under-determined systems
   i. Least squares problem (under constrained, less data than unknowns)
   ii. From the normal equations using Moore-Penrose inverse
   iii. Using QR decomposition of the rectangular system
   iv. Using SVD
   v. Using optimization techniques

q. Solving nonlinear equations
   i. Bisection methods
   ii. Fixed point iteration
   iii. Newton's method for nonlinear systems

r. Introduction to Wavelets

s. Numerical integration (quadrature) procedures:
   i. Trapezoidal rule
   ii. Midpoint rule
iii. Simpson’s rule  
iv. Gaussian quadrature  
v. Romberg integration  
vi. Integration in higher dimension  
t. Numerical differentiation using Taylor series  
u. Brief review of differential equations, types of boundary conditions, analytical solution procedures and model problems  
v. Introduction to finite difference approach; model problems in 1-D; and Lax equivalence theorem  
w. Introduction to finite element method; model problems in 1-D  
x. Brief review of integral equations and Green’s function