THE UNIVERSITY OF TEXAS AT DALLAS

# Numerical Methods in Engineering

## EE 6481

## Summer 2005

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## Target Audiences:

- Full-time graduate students in Electrical Engineering and Physics who use computational methods in their dissertation research
- Employees of local high-technology industry who regularly use computational methods and who want practical tools, but not a cookbook

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## Concepts/Tools to be Acquired in this Course:

- An understanding of the condition number of a problem. Examples of ill-conditioned problems include floating-point subtraction, finding multiple roots of a polynomial, and solving a system of linear equations with an ill-conditioned coefficient matrix.
- An understanding that algorithms outside the area of linear equations may be ill-conditioned. Examples include upward recursion for Bessel functions of the first kind, and finite-difference algorithms for ordinary differential equations applied outside of the algorithm's region of stability.
- An appreciation of the influences of the nature of the problem to be solved, the properties of floating-point arithmetic, the architecture of available computers, and algorithm design on the feasibility and accuracy of numerical computations.

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## Textbooks:

- Modern Mathematical Methods for Physicists and Engineers, by Prof. Cantrell,

published by Cambridge University Press (ISBN 0-521-59827-3) (Required). There is a UTD Web site for this book with a discussion area.
● Selected chapters from Numerical Recipes (in C, FORTRAN or Pascal), by Press, Teukolsky, Vetterling and Flannery (Recommended).

## Syllabus:

1. Floating-point arithmetic:
    - Floating-point representations
        - General properties
        - IEEE-754
            - 32-bit and 64-bit formats
            - Denormalized numbers
            - NaNs and other special values
            - Floating-point exception handling
        - CRAY
    - Rounding methods
    - Floating-point operations (+, -, X, /)
    - Catastrophic cancellation due to subtraction; introduction to the concept of condition number

2. Evaluation of functions
    - Evaluation of polynomials; illustration of catastrophic cancellation
    - Evaluation of multiple roots of polynomials (example of ill-conditioned problem; practical approaches)
    - Evaluation of partial sums of series
        - Alternating vs. same-sign; natural vs. reversed order
        - Kahan's algorithm
    - Recursive evaluation of functions
        - Integral \int_0^1 x(1+x)^{-n} dx
        - J_n(x): Miller's method, continued fractions, and more
        - Clebsch-Gordan (or 3-j) coefficients

3. Lightning survey of computer architectures
    - Von Neumann (model embedded in C and other languages)
    - Hierarchical memory; memory interleaving
    - CISC
    - Pipelining; RISC architectures
        - Dependency analysis for computation on a pipelined machine
    - Vector architectures
        - CRAY
        - CONVEX C-series
        - Practical aspects of vectorization of scientific and engineering programs
    - Parallel architectures
        - CONVEX Exemplar
        - CRAY (X/MP, Y/MP, C-90)
        - Symmetric multiprocessors (Sun, others)
        - Practical aspects of parallelization of scientific and engineering programs
    - High-performance computing

        - Performance analysis, profiling, etc.
        - Benchmarking strategies

4. Basic concepts of computational linear algebra (some material is review)
    - Vector spaces; dimension and basis; R^n and C^n
    - Linear mappings; range and null space; matrices; rank-nullity theorem
        - Ordering of array elements in C and FORTRAN
        - Loop orderings in matrix multiplication
        - Sampling and interpolation as linear mappings
    - Systems of linear equations; Gaussian elimination
        - LU decomposition
        - Gaussian elimination/LU decomposition on pipelined, vector and parallel machines
        - Computation of bases of range and null space using LU decomposition
        - Diagonal dominance and non-singularity
        - Iterative methods
            - Basis for iterative methods: The contraction mapping theorem
            - Gauss-Seidel iteration
            - Successive over-relaxation
            - Krylov subspace methods
    - Inner products and norms for vectors and matrices
        - Orthogonality; QR decomposition
        - 3-term recurrence relations for orthogonal polynomials
        - Vector norms
        - Matrix norms; relation to vector norms
        - Condition number of a matrix
        - Accuracy of Gaussian elimination
    - The singular-value decomposition (SVD)
        - Computation of the SVD
        - Computation of the fundamental subspaces of a linear mapping A [range(A), null(A), range(A^T), null(A^T)]
        - Analysis of ill-conditioned linear systems using the SVD
        - Moore-Penrose pseudo-inverse; application to ill-conditioned linear systems
    - The linear-least-squares-fitting problem
        - Formulation; standard covariance analysis
        - Condition number for least-squares fitting; relation to condition number of normal matrix
        - Example of an ill-conditioned least-squares problem: Fitting to a polynomial
    - The matrix eigenvalue-eigenvector problem
        - Bounds on matrix eigenvalues
        - Perturbations of the eigenvalue spectrum
        - Eigenvalues and eigenvectors of tridiagonal and Hessenberg matrices
        - Recursive transformation of a Hermitian matrix to tridiagonal form; Lanczos recursion
        - Survey of practical algorithms and packages

5. Numerical integration
    - Rectangle rule, trapezoidal rule, and Simpson's rule
    - Newton-Cotes methods
    - Practical adaptive-quadrature algorithms

    - Gaussian quadrature methods

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6. Finite-difference methods for ordinary differential equations
    - Solution of linear, homogeneous difference equations with constant coefficients
    - Survey of methods for deriving finite-difference algorithms
    - Stability analysis of finite-difference methods
        - Euler, backward Euler
        - Midpoint
        - Trapezoidal
        - Midpoint-trapezoidal predictor-corrector
        - Runge-Kutta methods
        - Adams-Moulton methods
        - Adams-Bashforth methods
    - Methods for stiff equations
        - Backward Euler
        - Gear's methods
    - Methods for linear systems of ODEs in which the coefficient matrix has purely imaginary eigenvalues
    - Finite-difference methods as digital filters: Transfer-function analysis
    - Boundary-value problems for ODEs

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7. Numerical methods for partial differential equations
    - First-order quasilinear PDEs
        - Method of characteristics
            - Burgers' equation
            - Shock waves and characteristics
            - Stability analysis of explicit FD methods: Transfer function, von Neumann's method, matrix method
            - Weighted-differencing methods; upwind differencing
            - Implicit differencing schemes
        - Classification of second-order quasilinear PDEs
        - Hyperbolic PDEs
            - Method of characteristics (standard formulation)
            - Method of characteristics (matrix formulation)
            - Finite-difference schemes
            - Dispersion-relation analysis of finite-difference schemes
        - Parabolic PDEs
            - General approach: Discretization in space, leading to a system of ODEs in time
            - Explicit methods; stability analysis; stiffness of resulting system of ODEs
            - Implicit methods; stability analysis
                - Crank-Nicholson
                - Stiff methods
                - Incorporation of derivative boundary conditions in matrix method of stability analysis
                - Stability analysis using transfer functions
                - Predictor-corrector methods for nonlinear parabolic PDEs
                - Operator-splitting methods
            - Absorbing boundary conditions
            - Application of digital filtering to nonlinear parabolic PDEs

    - The paraxial-wave equation
      - Spectral and pseudo-spectral methods
      - Case study of laser-beam propagation in a nearly-resonant medium
      - Bidirectional propagation
    - Survey of finite-element methods
  - Elliptic PDEs
    - Finite-difference schemes
    - Iterative methods for solving linear systems
      - Jacobi, Gauss-Seidel
      - Successive over-relaxation
      - Conjugate gradients
    - Operator-splitting methods
    - Multigrid methods

8. Pseudorandom-number generators

9. The FFT