AER336: SCIENTIFIC COMPUTING (Spring 2006)

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Course Description

This course provides an introduction to numerical methods for scientific computation which are relevant to engineering problems. Topics addressed include interpolation, integration, linear systems, least-squares fitting, nonlinear equations and optimization, initial value problems, partial differential equations, and relaxation methods. The assignments make extensive use of MATLAB. Assignments also require knowledge of FORTRAN or C.

Textbook: *Introduction to Scientific Computing*
by C. F. Van Loan
2nd Edition, Prentice-Hall, 2000

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Assignments: Assignment #1, Due: January 31
Assignment #2, Due: February 9
Assignment #3, Due: March 2
Assignment #4, Due: March 16
Assignment #5, Due: March 30
Assignment #6, Due: April 11.

Marks: 5% for several mini assignments (bonus marks)
25% for the six assignments (listed above)
12.5% for term test #1, Date: February 14
12.5% for term test #2, Date: March 28
50% for final exam

All tests and exams are type X ("open book") and permit use of type 1 calculators.

Web Site: `http://oddjob.utias.utoronto.ca/dwz/`

Outline

1. **Introduction**
   - What is Scientific Computing?
   - Learning to Use MATLAB
2. **Interpolation**
   - Global Polynomial Interpolation
     * Lagrange Polynomials
   - Piecewise Polynomial Interpolation
     * Cubic Splines
3. **Integration**
   - Newton-Cotes Rules
     * Trapezoidal Method
     * Simpson's Method
   - Composite Rules and Adaptive Quadrature
   - Gauss Quadrature
   - Spline Quadrature
4. **Linear Systems of Equations**
   - LU Decomposition
     * Pivoting
5. **Least Squares Fitting**
   - Linear Regression
   - Normal Equations
   - QR Factorization
6. **Nonlinear Equations and Optimization**
   - Roots of Scalar Nonlinear Equations
     * Bisection Method
     * Newton's Method
     * Secant Method
   - Systems of Nonlinear Equations
   - Minimizing Univariate Functions
     * Golden Section Search

        - Newton's Method
    - Minimizing Multivariate Functions
        - Method of Steepest Descent
        - Newton's Method

7. **Numerical Solution of Ordinary Differential Equations**
    - Initial and Boundary Value Problems
    - Systems of ODEs and Higher-Order ODEs
    - Time Marching Methods
        - Representative Linear First-Order ODE
            - Exact Solution
        - Ordinary Difference Equations
            - Converting Time Marching Methods to Ordinary Difference Equations
            - Solution of Ordinary Difference Equations
        - Accuracy and Stability of Time Marching Methods
        - Linear Multistep Methods (LMMs)
            - Explicit and Implicit Euler Methods
            - Trapezoidal Method
            - Adams-Bashforth and Adams-Moulton Methods
        - Predictor-Corrector Methods
            - Heun's (MacCormack's) Method
            - Burstein Method
        - Runge-Kutta Methods

8. **Numerical Solution of Partial Differential Equations**
    - Finite-Difference Methods
        - Taylor Tables
        - Compact Schemes
    - Model Equations
        - Linear Convection (Advection) Equation
        - Linear Diffusion Equation
    - Semi-Discrete Approach and Reduction of PDEs to ODEs

9. **Relaxation Methods**
    - Classical Relaxation Methods
        - Point-Jacobi
        - Gauss-Seidel
        - Successive Overrelaxation (SOR)

References

- **Textbook**: *Introduction to Scientific Computing*, 2nd Edition, by C. F. Van Loan, Prentice-Hall, 2000.
- **Useful Reference**: *Fundamentals of Computational Fluid Dynamics*, by H. Lomax, T. H. Pulliam, and D. W. Zingg, Springer, 2001.
- *Analysis of Numerical Methods*, by E. Isaacson and H. B. Keller, Dover, 1966.
- *Numerical Methods for Scientists and Engineers*, by R. W. Hamming, Dover, 1973.
- *Computer Methods for Mathematical Computations*, by G. E. Forsythe, M. A. Malcolm, and C. B. Moler, Prentice Hall, 1977.
- *An Introduction to Numerical Computations*, by S. Yakowitz and F. Szidarovszky, Macmillan Publishing, 1989.
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- *Applied Numerical Methods for Digital Computation*, Fourth Edition, by M. L. James, G. M. Smith, J. C. Wolford, HarperCollins College Publishers, 1993.
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- *Numerical Methods*, Second Edition, by J. D. Faires and R. L. Burden, Brooks/Cole Publishing, 1998.
- *Numerical Analysis*, 7th Edition, by R. L. Burden and J. D. Faires, Brooks/Cole Publishing, 2000.