

ChE 730 Advanced Numerical Methods

Spring Semester, 2011

Instructor: Ray Y. K. Yang
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Time and Location: 3:00 - 4:15 pm, Tuesday & Thursday; Room 211 ESB.

Prerequisite: A background in elementary differential equations and basic numerical methods is required. Some prior experience in MATLAB is useful but not required.

Book Used: a) Brian Hahn and Daniel Valentine, *Essential MATLAB for Engineers and Scientists*, 4th Ed., Academic Press, 2010. (Required)
b) Copy of parts of the draft of *Numerical Methods for Differential Equations*, a book being prepared by the instructor, will be distributed.

Course Outline*:

1. Introduction
Reviews of Basic MATLAB; Reviews of Relevant Methods for Solving Linear and Nonlinear Algebraic Equations; Deterministic Models and Mathematical Modeling.
2. Methods for Initial-Value Type Ordinary Differential Equations (ODEs)
Qualitative Theory of ODEs; Multiple-Step Formulas; Predictor-Corrector Methods; Runge-Kutta Methods; Numerical Stability; Methods for Stiff ODEs.
3. Methods for Initial-Value Type Partial Differential Equations (PDEs)
Qualitative Theory of PDEs; Finite-Difference Methods for Parabolic PDEs; Methods for Non-Dirichlet Boundary Conditions; Other Methods for Parabolic PDEs; Methods for Hyperbolic PDEs.
4. Methods for Boundary-Value Type Ordinary Differential Equations (ODEs)
Shooting Methods; Finite-Difference Methods; Other Methods.
5. Methods for Boundary-Value Type Partial Differential Equations (PDEs)
Finite-Difference Methods for Elliptic PDEs; Two-Dimensional Parabolic PDEs.
Other methods.

* Presentation of the topics may not follow exactly the same order as listed above.

Assessment:

1. Homework problems/projects: 80%
2. Two-hour final examination: 20%

Books on Reserve in Evansdale Library:

1. L. Lapidus and J. H. Seinfeld, "Numerical Solution of ODEs," Academic Press (1971).
2. S. C. Chapra and R. P. Canale, "Numerical Methods for Engineers," 6th Ed., McGraw-Hill (2010).
3. D. V. Von Rosenberg, "Methods for Numerical Solutions of PDEs," Elsevier (1969).
4. G. J. Borse, "Numerical Methods with MATLAB," PWS (1997).
5. S. C. Chapra, "Applied Numerical Methods with MATLAB for Engineers and Scientists," McGraw-Hill (2005).
6. B. H. Hahn and D. T. Valentine, *Essential MATLAB for Engineers and Scientists*, 4th Ed., Academic Press, 2010 [electronic resources].

Other Reference Books on Numerical Methods:

1. T. J. Akai, "Applied Numerical Methods for Engineers," Wiley (1994).
2. B. A. Finlayson, "Nonlinear Analysis in Chemical Engineering," McGraw-Hill (1980).
3. B. Carnahan, H. A. Luther and J. O. Wilkes, "Applied Numerical Methods," Wiley (1969).
4. M. E. Davis, "Numerical Methods and Modeling for Chemical Engineers," Wiley (1984).
5. L. Lapidus, "Digital Computation for Chemical Engineers," McGraw-Hill (1962).
6. L. Lapidus and G. F. Pinder, "Numerical Solution of PDEs in Science and Engineering," Wiley (1982).
7. S. Nakamura, "Applied Numerical Methods with Software", Prentice Hall (1991).
8. W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, "Numerical Recipes --The Art of Scientific Computing," Cambridge University Press (1986).
9. W. F. Ramirez, "Computational Methods for Process Simulation", Butterworths (1989).
10. J. R. Rice, "Numerical Methods, Software, and Analysis" 2nd Ed., Academic Press (1993).
11. G. D. Smith, "Numerical Solution of PDEs," Oxford Univ. Press (1965).
12. J. Villadsen and M. L. Michelsen, "Solution of Differential Equation Models by Polynomial Approximation," Prentice Hall (1978).
13. A. Constantinides and N. Mostoufi, "Numerical Methods for Chemical Engineers with MATLAB Applications," Prentice Hall, 1999.

Social Justice Statement:

West Virginia University is committed to social justice. I concur with that commitment and expect to foster a nurturing learning environment based upon open communication, mutual respect, and non-discrimination. Our University does not discriminate on the basis of race, sex, age, disability, veteran status, religion, sexual orientation, color or national origin. Any suggestions as to how to further such a positive and open environment in this class will be appreciated and given serious consideration. If you are a person with a disability and anticipate needing any type of accommodation in order to participate in this class, please advise me and make appropriate arrangements with Disability Services (293-6700).