A Course on

DIGITAL COMPUTATIONS FOR CHEMICAL ENGINEERS

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A NEW GRADUATE COURSE on *"Digital Computations for Chemical Engineers"* has been developed recently by the author at Auburn University. The major objective of the course is to introduce to the student the theory and application of the polynomial (or functional) and finite difference approximations in the solution of mathematical models in ChE. Brief discussions on the use of these approximation techniques in the analysis of experimental data are also included.

The contents of the course are distributed into three broad topics: I. Introduction to polynomial approximation and finite difference, II. Numerical solution of ordinary differential equations (ODE), and III. Numerical solution of partial differential equations (PDE). The progression of the course follows the sequence given in Table I, which lists the breakdown of the course in parts and chapters. The course is divided into two three-credit-hour quarter-courses. The first three-fifths of the topics is covered in ChE 600, "ChE Analysis," and the remainder in ChE 650, "Special Topics in ChE." As Seen in Table I, the course puts less emphasis on the computational solution of system of linear and nonlinear algebraic equations as well as the boundary value problems in ODE. These topics are discussed only briefly within Topics II and III, and are covered in more depth in courses on computer aided process design and optimal control of process systems. Although a number of the recent textual references are given in Table II, a single textbook which is suitable for the course does not exist. Consequently, lecture notes have to be prepared for the course. However, note-taking during the lectures is eliminated through the use of detailed handouts on most of the lecture material.

Referring to Tables I and II, a few remarks on the course contents and the source of the course material are as follows. Topic I contains a concise introduction of polynomial approximation and finite difference, with special emphasis on their applications to the computational analysis of experimental data. The problem of finding a polynomial of a specified degree to approximate a known function given either in an analytical form or as sets of discrete data is considered. The important questions related to this problem are discussed from the approximation theory[1] using finite difference table and associated linear symbolic operators.[2] The actual lectures follow much of the standard material on polynomial approximation and finite difference from reference texts 2, 5, 6, 10, and 12 in Table II. The reported results on the development and implementation of computational algorithms on the topic subject from such periodicals as *Communications of the Association for Computing Machine (CACM)* and *Numerische Matermatik* are discussed. An index by subject on these algorithms published in 1960-1970 is conveniently available in the reference text 4 in Table II. Weekly homework problems on applying the lecture material to such problems as the interpolation of discrete data of vapor pressure versus temperature, the differential and integral methods of kinetic analysis from experimental data are given. A special problem on the practical application of spline approximation to the analysis of thermodynamic data[3, 4] is also assigned.

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TABLE I.
A TOPICAL OUTLINE OF THE COURSE

I. INTRODUCTION TO POLYNOMIAL APPROXIMATION AND FINITE DIFFERENCE:

(1) Topics—polynomial approximation, finite difference, interpolation and extrapolation, numerical differentiation and integration, orthogonal polynomials and quadrature formulas.

(2) Selected Application—analysis of thermodynamic data by the spline approximation technique.

II. NUMERICAL SOLUTION OF ORDINARY DIFFERENTIAL EQUATIONS (ODE):

(1) Topics—fundamental concepts, Runge-Kutta and allied single-step formulas, predictor-corrector methods, stability of multistep and Runge-Kutta methods, stiff differential equations.

(2) Selected Application—digital parameter estimation of complex chemical reaction systems.

III. NUMERICAL SOLUTION OF PARTIAL DIFFERENTIAL EQUATIONS (PDE):

Chapter III-1. Fundamental Concepts

Fundamental notations, first and second order PDE, system of first order PDE, initial and boundary conditions, finite difference approximation, functional approximation, further mathematical background, questions raised.

Chapter III-2. Methods of Lines (MOL) and Method of Characteristics (MOC)

Introduction, basic concepts in the MOL, inverse methods, consistence, convergence and stability, MOL for parabolic, hyperbolic and elliptic PDE, method of characteristics, other extensions.

Chapter III-3. Finite Difference Solution of Parabolic Equations

Introduction, model parabolic PDE, explicit and implicit finite difference approximations, consistency and convergence, heuristic, Von Neumann and matrix stability concepts, some extensions, solution of finite difference approximations, composite solutions-global extrapolation and local combinations, explicit and implicit methods for two- and three-dimensional problems—alternating direction, local one dimension, fractional splitting and hopscotch methods, other extensions.

Chapter III-4. Finite Difference Solution of Hyperbolic Equations

Introduction, model hyperbolic PDE, first order hyperbolic PDE, first order vector and vector conservative hyperbolic PDE, two- and three-dimensional hyperbolic PDE, second order model hyperbolic PDE, other extensions.

Chapter III-5. Finite Difference Solution of Elliptic Equations

Introduction, model elliptic PDE, finite difference approximations of two- and three-space dimensional problems, solution of finite difference approximations—direct methods, iterative methods, sparse matrix techniques, composite solutions and other methods, conversion of elliptic to hyperbolic or parabolic equation, other extensions.

Chapter III-6. Variational, Least-Square and Moment Methods

Introduction, variational principles, Rayleigh-Ritz method and extensions, variational solution of parabolic, hyperbolic and elliptic PDE, dynamic programming and invariant imbedding approach, least-square and moment methods, comparison with other methods, further extensions.

Chapter III-7. Galerkin Methods

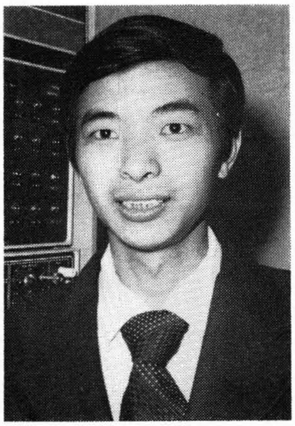
Introduction, general features of Galerkin methods, solution of parabolic PDE-continuous-time Galerkin, Crank-Nicholson Galerkin, hopscotch-Galerkin, local one dimensional Galerkin methods, solution of hyperbolic and elliptic PDE, comparison with other methods, further extensions.

Chapter III-8. Collocation Methods

Introduction, collocation points and approximating polynomials, the line collocation, orthogonal collocation and finite element collocation methods, solution of parabolic, hyperbolic and elliptic PDEs, comparison with other methods, further extensions.

Chapter III-9. Finite Element Methods

Introduction, variational finite element methods, weighted-residual finite element method, element types and basis functions, the time dimension, finite element matrix structure and storage schemes, solution of linear equations in finite element analysis, solution of parabolic PDE-finite element heat and mass transfer analysis,



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solution of hyperbolic PDE, solution of elliptic PDE-finite element method and fluid flow problems, comparison with other methods, further extensions.

Chapter III-10. Practical Considerations in Polynomial (Functional) Approximation Methods

Introduction, continuous and discrete methods of weighted residuals, the selection of weighting functions, the selection of approximating functions, the problem specific polynomial approach, further extensions.

Chapter III-11. Selected Applications

Introduction, solution of Navier-Stokes equations, solution of problems of adsorption, chromatography and ion exchange columns, solution of oil and gas reservoir problem, solution of phase change and related moving boundary problems, solution of water resources problems, solution of population balance equations, solution of catalytic fixed bed reactor problem.

ORDINARY DIFFERENTIAL EQUATIONS

IN TOPIC II, the fundamental concepts and definitions in numerical solution of ODE are introduced. The practical considerations in numerically solving ODE such as stability, accuracy and computational efficiency are also considered. Here, the important material from three recent books 4, 7, and 8 in Table II is briefly discussed, and supplemented with the excellent monograph on stiff ODE edited by Willoughby (see Table II). The specific lectures begin with some basic techniques for deriving integration formulae for ODE and related terminologies. The Taylor series expansion is used first to derive the simplest Euler's formula and the concept of trunction error. The forward and backward Taylor series expansions are then combined to derive the midpoint rule. These two integration formulae provide the typical examples for defining the explicit as well as the single-step and multi-step methods. Next, both the Euler's formula and midpoint rule are derived by using numerical differentiation and/or integration formulae. The integration of the ODE by the trapezoidal rule gives the modified Euler's formula, which serves as an example for introducing the implicit method. The combined use of the Euler formula, the original ODE and the modified Euler's formula suggests the family of predictor-evaluation-corrector-evaluation (PECE) methods. A generalized, linear, multi-step differential-difference equation with constant coefficients is then defined to summarize the preceding discussions concisely and to encompass all previous integration formulae within the same framework. The course is continued with the illustration of the concept of order by deriving, for example, the second-order Adams-Bashforth predictor equation from polynomial approximation. With these preliminaries in hand, the next step in the course is to introduce the generalized Adams-Bashforth formaulae, the Adams-Moulton's forms and the Nystrom explicit forms, etc. The well-known Runge-Kutta processes are discussed in a vector-matrix form[5] and applied to many homework problems. At this time, a special topic on the parameter estimation in ODE from experimental data is given. A generalized nonlinear least-square, curve-fitting procedure[6, 7] is introduced and a problem of computerized kinetic analysis in the batch fermentation of penicillin is assigned to the students. The effectiveness and comparison of different methods in solving ODE are then presented.[8, 9] Topic II is concluded with lectures on the occurrence of stiff ODE in chemical engineering,[10] and several efficient integration packages for solving stiff ODE such as by Gear.[11] Finally, many interesting papers on stiff ODE from the reference text 15 in Table II are discussed.

PARTIAL DIFFERENTIAL EQUATIONS

ALTHOUGH A CONSIDERABLE amount of the latest knowledge on the numerical solution of PDE by polynomial (or functional) approximation has been reviewed in reference texts 3, 13, and 17 in Table II, such texts on the numerical solution of PDE by finite difference as 1, 6, 9-11, 14-16 in Table II contain only that literature published before 1970. A suitable book covering the up-to-date information of both types of approximations does not exist. Thus, the lecture-notes for Topic III are mostly the original developments in the course. An outline in chapters and sections has been included in Table I. It should be mentioned that the developments of

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these notes would not be possible without the encouragement, support and participation of Professor Leon Lapidus of Princeton University. The computer listing of the latest publications as well as the hundreds of reference reports and reprints on the numerical solution of PDE given by Professor John H. Giese of University of Delaware have been most helpful. In addition, a number of excellent literature reviews and the latest developments on the subjects on Topic III have been found in several recent doctoral dissertations. For example, studies which are concerned with the method of line for PDE[12] (Chapter III-2), the composite numerical solution of PDE[13] (Chapter III-3 to III-5), finite element method for heat conduction analysis[14] and fluid flow problems[15] (Chapter III-9), collocation method for the analysis of chromatographic system[16] (Chapter III-8) have been reported. While further discussions on the course contents and source material for Topic III are not possible within the limits of this article, a detailed write-up and specific subject references on the numerical solution of PDE can be obtained by writing to the author.

TABLE II. SOME TEXTUAL REFERENCES OF THE COURSE

1. Ames, W. F., "Numerical Solution of Partial Differential Equation," Barnes & Nobles (1969).
2. Dahlquist, G., A. Bjorck, & N. Anderson, "Numerical Methods," Prentice-Hall (1974).
3. Finlayson, B. A., "The Method of Weighted Residuals and Variational Principles," Academic Press (1972).
4. Gear, C. W., "Numerical Initial Value Problems in Ordinary Differential Equations," Prentice-Hall (1971).
5. Issacson, I., & H. B. Keller, "Analysis of Numerical Methods," Wiley (1966).
6. Lapidus, L., "Digital Computations for Chemical Engineers," McGraw-Hill (1962).
7. Lambert, J. D., "Computational Methods in Ordinary Differential Equations," Wiley (1973).
8. Lapidus, L., & J. H. Seinfeld, "Numerical Solution of Ordinary Differential Equations," Academic Press (1971).
9. Mitchell, A. R., "Computational Methods in Partial Differential Equations," Wiley (1969).
10. Ralston, A., & H. S. Wilf, Editors, "Mathematical Methods for Digital Computers," Wiley, Vol. I (1960), and Vol. 2 (1967).
11. Richtmyer, R. D., & K. W. Morton, "Difference Methods for Initial Value Problems," 2nd Edition, Interscience (1967).
12. Rosenbrock, R. H., & C. Storey, "Computational Techniques for Chemical Engineers," Pergamon Press (1966).
13. Strang, G., & G. Fix, "An Analysis of the Finits Element Method," Prentice-Hall (1973).
14. Varga, R. S., "Matrix Iterative Analysis," Prentice-Hall (1962).
15. Willoughby, R. A., Editor, "Proceedings of International Symposium on Stiff Differential Systems," Wilbad, Germany, Plenum Press (1974).
16. Young, D. M., "Iterative Solution of Large Linear Systems," Academic Press (1972).
17. Zienkiewicz, O. Z., "The Finite Element Method in Engineering Science," 2nd Edition, McGraw-Hill (1967).

A generalized non-linear least square, curve-fitting procedure is introduced and a problem of computerized kinetic analysis in the batch fermentation of penicillin is assigned . . . the effectiveness and comparison of different methods in solving ODE are then presented.

WORK REQUIREMENTS

A BRIEF REMARK about the course requirement may be of interest here. Homework problems are assigned to the class weekly. Each student is required to conduct an independent course project and to submit a term paper which includes: (a) a concise literature survey of the most important publications in the topic chosen, (b) a critical analysis of the computational techniques involved and a proper evaluation of the "state of the art," and (c) suggestions for further investigations as well as a preliminary analysis of the feasibility of the proposed research areas. Since no course examinations are given, this provides more opportunities for each student to pursue the specific subjects of interest. Typical subjects on the term projects chosen by the class during the last year include the method of characteristics, the method of lines, the analysis of chromatographic system, the collocation method, and the extrapolation technique for the solution of PDE and nonlinear algebraic equations. It is encouraging to mention that several of these projects conducted by the class in the course have led to some quite original research

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propositions. What is perhaps the most encouraging of all is the interest in this course and the constructive criticism by the class.

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4. Klaus, R. L., & H. C. Van Ness, AIChE J., *13*, 1132 (1967).
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11. Gear, C. W., Comm. ACM, *14*, 185 (1971).
12. Larson, L., "Automatic Solution of Partial Differential Equations," Ph.D. Thesis, University of Illinois (1972).
13. Burgess, W. P., "Composite Numerical Solution of PDE," Ph.D. Thesis, Princeton University (1971).
14. Laskaris, T. E., "Finite Element Analysis of Several Compressible and Uncompressible Viscous Flow Problems," Ph.D. Thesis, Rensselaer Polytechnic Institute (1974).
15. Chakrabarti, S., "Approximations in Finite Element Heat Conduction Analysis," Ph.D. Thesis, University of Pittsburgh (1974).
16. Woodrow, P. T., "Analysis of Chromatographic Systems Using Orthogonal Collocation," Ph.D. Thesis, Rensselaer Polytechnic Institute (1974).

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'67-9 and cited ten or more times.

10. **Papers/professor: Works published in the '67-9 period divided by the number of professors, publishing or not, in the departments in that period.**
11. **Citations/paper: Total citations divided by the number of '67-9 works (impact factor).**
12. **Papers with 0-4 citations: '67-9 works with through four total citations.**
13. **1970 Rating of Graduate Programs: Detailed data of Roose and Andersen study on rankings of departments of ChE kindly supplied by Andersen.**
14. **Ph.D.'s graduated: Ph.D.'s graduated per year during '67-9.**
15. **Ph.D's/professor: Ph.D.'s graduated per faculty member per year in '67-9.**
16. **Lifetime citations/professor: The number of citations, including self-citations, to all works on which a faculty member is first or only author divided by the number of professors, publishing or not, in the literature cited.**
17. **Professors/school: The number of professors, publishing or not, in the literature cited divided by number of schools (21).**

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9. Matheson, A. J., *Chemistry in Britain, 8*, 202-10, (1972).
10. *American Chemical Society Directory of Graduate Research*, American Chemical Society, Washington, D. C., (1971).
11. *Science Citation Index*, Institute for Scientific Information, Philadelphia, (1965-72).
12. Hagstrom, W. O., "Inputs, Outputs and the Prestige of American University Science Departments," Paper delivered at the American Association for the Advancement of Science, Chicago, Ill., (Dec. 28, 1970).
13. Unpublished work supplied by Malin of the Institute for Scientific Information.