Then eqns. (11), (12), (13), etc., are linear implicit equations which may be solved successively to give $\mathbf{k}_r$, $\mathbf{l}_r$, $\mathbf{m}_r$, etc. We shall say that such a process has q stages if R_q is not zero, but all succeeding R are zero.

By a straightforward but tedious calculation it is possible to expand $\mathbf{x}'_r - \mathbf{x}'_{r-1}$ in eqn. (14) as a power series in h_r, and to compare this with the Taylor's series. It is found that the following equations must be satisfied in a two-stage process in order to ensure correspondence between the early terms of both series:

$$h_r: \quad R_1 + R_2 = 1 \tag{15}$$

$$h_r^2: \quad R_1a_1 + R_2(a_2 + b_1) = \tfrac{1}{2} \tag{16}$$

$$h_r^3: \begin{cases} R_1a_1^2 + R_2[a_2^2 + (a_1 + a_2)b_1] = \tfrac{1}{6} & (17)\\ R_2(a_2c_1 + \tfrac{1}{2}b_1^2) = \tfrac{1}{6} & (18)\end{cases}$$

$$h_r^4: \begin{cases} R_1a_1^3 + R_2[a_2^3 + (a_1^2 + a_1a_2 + a_2^2)b_1] = \tfrac{1}{24} & (19)\\ R_2a_2(a_2c_1 + \tfrac{1}{2}b_1^2) = \tfrac{1}{24} & (20)\\ R_2(a_1a_2c_1 + a_2^2c_1 + a_2b_1c_1 + a_1b_1^2) = \tfrac{1}{24} & (21)\\ R_2(\tfrac{1}{2}a_2c_1^2 + \tfrac{1}{6}b_1^3) = \tfrac{1}{24}. & (22)\end{cases}$$

In these equations there are six adjustable constants, a_1, a_2, b_1, c_1, R_1 and R_2. It follows that, at best, agreement can be obtained up to terms in h^3, leaving an error $0(h^4)$. Two further conditions may then be applied.

As an example, one possible solution of eqns. (15) to (18), with truncation error $0(h^4)$, is

$$a_1 = 1 + \sqrt{6}/6 = 1\cdot408\ 248\ 29 \tag{23}$$

$$a_2 = 1 - \sqrt{6}/6 = 0\cdot591\ 751\ 71 \tag{24}$$

$$b_1 = c_1 = \{-6 - \sqrt{6} + \sqrt{[58 + 20\sqrt{6}]}\}/(6 + 2\sqrt{6}) = 0\cdot173\ 786\ 67 \tag{25}$$

$$R_1 = -0\cdot413\ 154\ 32 \tag{26}$$

$$R_2 = 1\cdot413\ 154\ 32. \tag{27}$$

The function corresponding to eqn. (5) is

$$\psi_i(t) = \frac{1 + k_it - \frac{2}{3}(k_it)^2}{1 + 2k_it + \frac{5}{6}(k_it)^2} \tag{28}$$

which tends to $-0\cdot8$ as $t \to \infty$. It can be shown that there is no two-stage process with truncation error $0(h^4)$ for which $\psi_i(t) \to 0$ as $t \to \infty$.

Many alternative processes can be developed on the lines just given. If stability is the first consideration, it is possible to have a two-stage process for which $\psi_i(t) \to 0$ as $t \to \infty$, provided that a truncation error $0(h^3)$ is acceptable. An example is obtained with

$$a_1 = a_2 = 1 - \sqrt{2}/2,\ b_1 = (\sqrt{2} - 1)/2,\quad c_1 = 0,\ R_1 = 0,\ R_2 = 1. \tag{29}$$

Finally, if the constants are allowed to be complex, it is possible to obtain further processes. For example, consider the process defined by

$$\mathbf{k}_r = h_r\{\boldsymbol{\phi}(\mathbf{x}'_{r-1}) + a_1\mathbf{A}(\mathbf{x}'_{r-1})\mathbf{k}_r\} \tag{30}$$

$$\mathbf{x}'_r = \mathbf{x}'_{r-1} + \mathscr{R}R_1\mathbf{k}_r \tag{31}$$

with $$a_1 = \tfrac{1}{2}(1 + i),\ R_1 = 1. \tag{32}$$

This has a truncation error $0(h^3)$, and gives

$$\psi_i(t) = \frac{1}{1 + k_it + \frac{1}{2}(k_it)^2}. \tag{33}$$

Unfortunately the amount of work involved in the solution will be roughly quadrupled by the use of complex numbers.

Conclusion

The processes described above have been explored only cursorily, and it is hoped that this note may stimulate others to investigate their possibilities.

References

CRANK, J., and NICOLSON, P. (1947). "A practical method for numerical evaluation of solutions of partial differential equations of the heat-conduction type," *Proc. Camb. Phil. Soc.*, Vol. 43, pp. 50–67.

KOPAL, Z. (1955). *Numerical analysis*, pp. 211, 212 (Chapman and Hall).

Book Review

Digital Computation for Chemical Engineers, by L. LAPIDUS, 1962; 407 pp. (London: *McGraw-Hill Publishing Co. Ltd.*, 89s; New York: *McGraw-Hill Book Co. Inc.*)

This is another book mainly about computational methods in which the author has set out to describe those areas of computer mathematics which are of importance to the chemical engineer. Unlike most texts on this subject we find that the numerical examples have been collected and placed at the end of each chapter. Almost all these examples have been processed on digital computers of one sort or another, and machine times are given together with the programming system used. Lectures have been given on this material to undergraduate and graduate engineers and also to technical personnel in the chemical industry. About one-fifth of the book is devoted to worked examples. There are over 450 references.

Chapter 1 gives a brief introduction to the digital computer. Chapter 2 deals with polynomial approximation and includes interpolation, integration and differentiation. For equally spaced data, operators are used to derive Newton's forward and backward formulae, Gauss's forward and backward central-difference formulae, Stirling's, Bessel's and Everett's formulae. The throwback of higher differences is discussed. The Lagrangian formula for unequal intervals is derived and discussed. Numerical differentiation is treated at similar length to interpolation. The Newton–Cotes formulae for integration are derived, and the elimination of error terms by extrapolation to zero interval using integration at two different intervals is presented. Integration at unequally spaced intervals is considered and the formulae of Gauss for a finite interval of integration and for singly and doubly infinite limits are given. Quadrature formulae with various weighting functions are also mentioned. One of the main examples at the end of this chapter is the consideration of

$$I_{a,b} = \int_a^b (1 + 10x^2)^{-1} dx$$

and the comparison of the efficiency for various a and b of the Trapezoidal rule and the methods of Simpson, Weddle, Chebyshev and Legendre–Gauss. The author rightly points out that the ease of integration is closely connected with the limits a and b. A study of Table 2.6 shows that for $a = 0$, $b = 10$ and interval of integration $0 \cdot 1$, the Trapezoidal rule gives a more accurate answer than the application of Simpson's rule at the same interval. This unusual occurrence is not explained in the text but a closer examination reveals that the reason for this is to be found in the cancellation of error terms. Tables 2.5 and 2.8 show that $I_{0,1}$ for the Trapezoidal rule has a large positive error, whereas $I_{1,10}$ for the Trapezoidal rule has a similarly large negative error. The same cancellation does not take place with Simpson's rule.

Chapter 3 deals with ordinary differential equations, being mostly concerned with first-order equations and initial-value problems. There is a brief mention of boundary-value problems and a method for dealing with second-order linear equations with first derivatives absent. A selection of Runge–Kutta type methods is given and discussed. An unnecessarily complicated description and analysis of numerical stability is given. Repetition of the computation at a reduced interval is advocated for monitoring this type of integration procedure. No mention is made of the superior qualities of the Kutta–Merson procedure in this respect (vide *Numerical Solution of Ordinary and Partial Differential Equations*, L. Fox, Ed., Pergamon Press 1962, p. 24). Of the predictor-corrector methods, Milne's methods 1 and 2 and the Adams–Moulton method are treated. Only one application of the corrector equation is considered so that the formulae as given are of mixed type. There is thus no discussion of the convergence of the corrector equations and the stability analysis given is not, strictly speaking, applicable. There is no mention of the requirement for ultra-stable formulae or of Chebyshev methods of integration.

Chapter 4 deals with linear, second-order, partial differential equations. The treatment is fairly full and up to date. For the elliptic-type equations in two dimensions, the finite-difference approximations are developed. Methods of solution include direct solution and the iterative methods of successive over-relaxation, and Peaceman and Rachford's alternating-direction procedure. Curved boundaries are treated. The method of characteristics and finite-difference representation are both discussed for hyperbolic equations.

Chapter 5 is on linear algebra and begins with an account of matrices. Various elimination methods are discussed for equations. The eigenvalue problem is given a thorough treatment although important work which has appeared in the last three years is not included.

Chapter 6 deals adequately with roots of equations both polynomial and transcendental.

Chapter 7 gives methods of approximation for functions mostly of one variable. Included here are the least-squares fit and Chebyshev approximation. There is some mention of continued fraction expansions.

The last chapter on optimization and control deals with linear programming, giving the simplex solution and a rather special, though important, case of the control problem. A linear, sampled-data system is considered in which the control variables are held constant between sampling instants. The mathematics is developed to enable the best control action to be calculated for a quadratic performance index. This last chapter is more mathematical than computational.

It is apparent from the above that the coverage of computational topics is fairly full and detailed. There is, however, not a great deal to justify the second part of the title. Admittedly the examples have a chemical background, but a drawback to this is the amount of descriptive matter which has to be included. The author's practice of collecting up worked examples at the end of each chapter does not really come off in the opinion of your reviewer. The inner workings of numerical formulae are not fully exposed by the tabulation of an array of results which again do not form a complete basis for comparison of the usefulness of alternative procedures.

An important omission from Chapter 2 is the function of the difference table in error detection.

The reviewer would have expected a more positive approach on the part of the author to the discussion of particular chemical engineering problems requiring special computational treatment. There are many such problems, for example in distillation. Again, there is the field of conventional control problems which might have received some attention in Chapter 3. The collection of a large number of unattached references at the end of each chapter is of doubtful value. A short bibliography giving a few selected references on particular topics would have been much more valuable and would have eliminated the need for perhaps three-quarters of the references.

In spite of the criticisms which have been made above, the book is to be recommended to chemical engineers. There is no alternative available and the standard of presentation of the mathematics is high, as is the printing.

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