A high-order Crank–Nicholson technique for solving differential equations

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A generalized Crank–Nicholson technique is given for the solution of simultaneous first-order linear time-invariant differential equations. The method proposed is inherently stable for any time interval h, gives correct solutions for any h as $t \to \infty$ for polynomial type time inputs and has a truncation error of $O(h^5)$. It is especially suitable for the solution of large systems of differential equations.

Equations of the type

$$\dot{x} = Ax + Bu(t)\,,\; x(0) = x_0 \tag{1}$$

occur often in engineering and physics and it is therefore very desirable to have a fast efficient method for obtaining solutions especially when the number of equations is large. Standard methods of solution such as the Runge–Kutta method are normally unsatisfactory especially when there is a wide distribution of eigenvalues in the matrix A (which is often the case) because of instability problems (Rosenbrock and Storey 1966). This problem has been recently studied by Henrici (1964) in a recent review article in which he investigated a number of classical numerical techniques as well as some recent modified techniques with respect to stability.

Proposed method

Let x_t be the solution of equation (1) at time t, u_t be the value of $u(t)$ at time t and h be an increment in the time interval. Then x_{t+h} and x_t may be expressed in Taylor series as follows:

$$x_{t+h} = x_t + h\dot{x}_t + \frac{h^2}{2}\ddot{x}_t + \frac{h^3}{6}\dddot{x}_t + \frac{h^4}{24}\ddddot{x}_t \tag{2}$$

$$x_t = x_{t+h} - h\dot{x}_{t+h} + \frac{h^2}{2}\ddot{x}_{t+h} - \frac{h^3}{6}\dddot{x}_{t+h} + \frac{h^4}{24}\ddddot{x}_{t+h} \tag{3}$$

leaving a truncation error of order h^5.

Subtracting equation (3) from equation (2) and substituting for equation (1) gives:

$$\begin{aligned} x_{t+h} - x_t = {} & \frac{h}{2}(Ax_t + Bu_t) + \frac{h}{2}(Ax_{t+h} + Bu_{t+h}) \\ & + \frac{h^2}{4}(A^2x_t + ABu_t + B\dot{u}_t) + \\ & - \frac{h^2}{4}(A^2x_{t+h} + ABu_{t+h} + B\dot{u}_{t+h}) + \\ & + \frac{h^3}{12}(A^3x_t + A^2Bu_t + AB\dot{u}_t + B\ddot{u}_t) + \\ & + \frac{h^3}{12}(A^3x_{t+h} + A^2Bu_{t+h} + AB\dot{u}_{t+h} + B\ddot{u}_{t+h}) + \\ & + \frac{h^4}{48}(A^4x_t + A^3Bu_t + A^2B\dot{u}_t + AB\ddot{u}_t + B\dddot{u}_t) + \\ & - \frac{h^4}{48}(A^4x_{t+h} + A^3Bu_{t+h} + A^2B\dot{u}_{t+h} \\ & \qquad + AB\ddot{u}_{t+h} + B\dddot{u}_{t+h}). \end{aligned} \tag{4}$$

On solving for x_{t+h}, the following equation is obtained:

$$\begin{aligned} x_{t+h} = {} & \left(I - \frac{h}{2}A + \frac{h^2}{4}A^2 - \frac{h^3}{12}A^3 + \frac{h^4}{48}A^4\right)^{-1} \\ & \left(I + \frac{h}{2}A + \frac{h^2}{4}A^2 + \frac{h^3}{12}A^3 + \frac{h^4}{48}A^4\right)x_t + \\ & + \left(I - \frac{h}{2}A + \frac{h^2}{4}A^2 - \frac{h^3}{12}A^3 + \frac{h^4}{48}A^4\right)^{-1} \\ & \left\{\left(I + \frac{h}{2}A + \frac{h^2}{6}A^2 + \frac{h^3}{24}A^3\right)\frac{h}{2}Bu_t + \right. \\ & + \left(I - \frac{h}{2}A + \frac{h^2}{6}A^2 - \frac{h^3}{24}A^3\right)\frac{h}{2}Bu_{t+h} + \\ & \left(I + \frac{h}{3}A + \frac{h^2}{12}A^2\right)\frac{h^2}{4}B\dot{u}_t + \\ & - \left(I - \frac{h}{3}A + \frac{h^2}{12}A^2\right)\frac{h^2}{4}B\dot{u}_{t+h} + \left(I + \frac{h}{4}A\right)\frac{h^3}{12}B\ddot{u}_t \\ & \left. + \left(I - \frac{h}{4}A\right)\frac{h^3}{12}B\ddot{u}_t + \frac{h^4}{48}B\dddot{u}_t - \frac{h^4}{48}B\dddot{u}_{t+h}\right\}. \end{aligned} \tag{5}$$

If the right-hand side of equation (5) is now expanded as a power series in hA, it may readily be verified that the $\frac{h^4}{48}A^4$ terms can be omitted without increasing the truncation error of $O(h^5)$.

The proposed procedure to solve equation (1) becomes therefore

$$x_{t+h} = \left(I - \frac{h}{2}A + \frac{h^2}{4}A^2 - \frac{h^3}{12}A^3\right)^{-1}\left(I + \frac{h}{2}A + \frac{h^2}{4}A^2 + \right.$$

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$$+\frac{h^3}{12}A^3\Big)x_t + \Big(I - \frac{h}{2}A + \frac{h^2}{4}A^2 - \frac{h^3}{12}A^3\Big)^{-1}$$
$$\Big\{\Big(I + \frac{h}{2}A + \frac{h^2}{6}A^2 + \frac{h^3}{24}A^3\Big)\frac{h}{2}Bu_t$$
$$+\Big(I - \frac{h}{2}A + \frac{h^2}{6}A^2 - \frac{h^3}{24}A^3\Big)\frac{h}{2}Bu_{t+h} +$$
$$+\Big(I + \frac{h}{3}A + \frac{h^2}{12}A^2\Big)\frac{h^2}{4}B\dot{u}_t +$$
$$-\Big(I - \frac{h}{3}A + \frac{h^2}{12}A^2\Big)\frac{h^2}{4}B\dot{u}_{t+h} + \Big(I + \frac{h}{4}A\Big)\frac{h^3}{12}B\ddot{u}_t +$$
$$+\Big(I - \frac{h}{4}A\Big)\frac{h^3}{12}B\ddot{u}_t + \frac{h^4}{48}B\dddot{u}_t - \frac{h^4}{48}B\dddot{u}_{t+h}\Big\}. \quad (6)$$

It is seen that equation (6) is just a generalization of the well-known Crank–Nicholson or trapezoidal rule of solution (Crank–Nicholson, 1947). However, the proposed method has a smaller truncation error $O(h^5)$ compared to the Crank–Nicholson method $O(h^3)$.

It may be readily verified that equation (6) is numerically stable for all values of h since the eigenvalues of the matrix

$$\wedge = \Big(I - \frac{h}{2}A + \frac{h^2}{4}A^2 - \frac{h^3}{12}A^3\Big)^{-1}$$
$$\times \Big(I + \frac{h}{2}A + \frac{h^2}{4}A^2 + \frac{h^3}{12}A^3\Big) \quad (7)$$

are all less than one in magnitude. This can be established as follows. Assume for the present that A has eigenvalues either distinct or repeated with non-degenerate eigenvectors. Then A may be written in the form

$$A = \Gamma\lambda\Gamma^{-1} \quad (8)$$

where Γ is the matrix of eigenvectors of A and λ is a diagonal matrix of eigenvalues of A. On substituting equation (8) into equation (7), the following result is obtained:

$$\wedge = \Gamma\Big(I - \frac{h}{2}\lambda + \frac{h^2}{4}\lambda^2 - \frac{h^3}{12}\lambda^3\Big)^{-1}$$
$$\times \Big(I + \frac{h}{2}\lambda + \frac{h^2}{4}\lambda^2 + \frac{h^3}{12}\lambda^3\Big)\Gamma^{-1} \quad (9)$$

which implies that the eigenvalues of $\wedge$ are given by

$$\frac{1 + \frac{h}{2}\lambda_i + \frac{h^2}{4}\lambda_i^2 + \frac{h^3}{12}\lambda_i^3}{1 - \frac{h}{2}\lambda_i + \frac{h^2}{4}\lambda_i^2 - \frac{h^3}{12}\lambda_i^3}, \; i = 1, 2, \ldots, n$$

where λ_i, $i = 1, 2, \ldots, n$ are the eigenvalues of A. These eigenvalues of $\wedge$ are all less than one in magnitude if $Re(\lambda_i) < 0$, $i = 1, 2, \ldots, n$ which is always the case if equation (1) represents a stable system. If A has repeated eigenvalues with degenerate eigenvectors this same result will be obtained on substituting the Jordan canonical form of A into equation (7). It may also be verified that the iterative procedure given by equation (6) will approach the correct solution values of equation (1) for any value of h (and not just for the case that $h \to 0$) as $t \to \infty$ for any input $u(t)$ of the form

$$u(t) = \sum_{n=0}^{m} \alpha_n t^n, \quad t \geqslant 0$$
$$= 0 \qquad , \; t < 0.$$

This includes many time-functions of physical interest such as step-function inputs and ramp-type function inputs. This is important because it, along with the truncation error of $O(h^5)$, implies that the solution of equation (1) will be relatively accurate for large values of h. Hence if the solution of equation (1) is desired only to a limited degree of accuracy (say $0{\cdot}1\%$), and this is often the case, then a large h can be chosen to solve it, thereby avoiding excessive computation time.

It should be noted that the method of solution proposed could be carried another stage giving a truncation error of $O(h^7)$. However, this is impractical for two reasons. Double-precision arithmetic must be used to calculate A^5 if the range of magnitudes of the elements of A is greater than about 50 on an 8-figure digital computer. Also computation time to obtain A^5 will increase the total computational time. This additional computational time will often offset any advantage of the higher-order process $O(h^7)$.

Numerical example

The following set of equations was solved using the above procedure (equation (6)) and compared with the 4th order Runge–Kutta method and the standard Crank–Nicholson method,

$$\dot{x} = Ax + Bu(t)\,, \; x(0) = 0$$

where $u(t)$ is an unit step-function and A and B are given below:

$A = (a_{i,j})$ where

$$a_{i,\,i} = -0{\cdot}05\,k^{i-1}\;, \; i = 1, 2, \ldots n$$
$$a_{i+1,\,i} = 0{\cdot}005\,k^{i-1}\,, \; i = 1, 2, \ldots (n-1)$$
$$a_{i,\,i+1} = 0{\cdot}01 \qquad, \; i = 1, 2, \ldots (n-1)$$
$$a_{n,\,i} = -0{\cdot}02 \qquad, \; i = 1, 2, \ldots (n-2)$$
$$a_{i,\,n} = 0{\cdot}002 \qquad, \; i = 1, 2, \ldots (n-2)$$

and $k = 1{\cdot}17$ when $n = 70$, $k = 1{\cdot}25$ when $n = 50$, $k = 1{\cdot}45$ when $n = 30$ and $k = 3{\cdot}00$ when $n = 10$.

$B = (b_i)$ where

$$b_i = 0\,, \; i = 1, 2, \ldots (n-1)$$
$$b_i = 1\,, \; i = n.$$

Table 1 gives a comparison of times required to solve this set of equations for different values of n on the

IBM 7094 II digital computer. In all cases the step-size chosen with the Runge–Kutta method was taken to be as large as possible to just maintain stability. The equations were solved to at least 4 figure accuracy in all cases.

It is seen that the proposed method is significantly faster than the Runge–Kutta and faster than the standard Crank-Nicholson method in this example. It should be noted, however, that the storage space required in using the proposed method is greater than in using more conventional techniques. Approximately $5n^2$ words (where n is the order of the matrix A) are required for the case that n is large with the proposed method as compared to the n^2 words required in the case of the Runge–Kutta method.

Conclusion

It is believed that the method described in this paper represents an efficient technique for solving large sets of linear time-invariant differential equations. Equations of the type

$$\dot{x} = (A + \phi(x, t))x + Bu(t)$$

where $||\phi(x, t)|| \ll ||A||$, and this includes many physical processes, may be similarly considered by taking $\phi(x, t)x$ as part of the forcing function input.

Table 1

Time required to solve $\dot{x} = Ax + Bu(t)$

ORDER OF MATRIX A	SOLUTION BY RUNGE–KUTTA	SOLUTION BY STANDARD CRANK –NICHOLSON	SOLUTION BY PROPOSED METHOD
$n = 10$	40 minutes	3 seconds	0·2 seconds
$n = 30$	360 minutes*	33 seconds	2·2 seconds
$n = 50$	900 minutes*	90 seconds	10 seconds
$n = 70$	1800 minutes*	180 seconds	26 seconds

* These times are estimated.

References

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Book Review

Library Planning for Automation, edited by Allen Kent, 1966; 195 pages. (London: *Macmillan*, 52s.)

Dr Stafford L. Warren, special assistant to the President of the USA, proposed the setting up in America of a National Science Library System covering periodical literature in science, engineering, social science and law. This was to comprise a series of regional centres to store, in microform, perhaps 30,000 to 50,000 periodicals in the subject fields covered and make them available to academic and other libraries as required. It was envisaged that computer systems would be developed to provide access via a complete storehouse on tapes of summaries, abstracts and citations, and also to permit rapid and precise reaction to user requirements.

In order to scrutinize the Warren proposal the *Council of Library Resources* met the cost of bringing together a panel of experts, representing library planners and publishers of periodicals, to consider three papers. These were an outline of the Warren proposal itself, a paper on microforms which examined the state-of-the-art in relation to costs and equipment, and one on the influence of automation on the design of a university library.

The present book consists of the proceedings of the panel meetings, with full discussions, and an added paper on the question of copyright. The papers are good but the discussion, rendered verbatim, is of very variable quality. It is by no means always to the point and is sometimes trivial in content. On the whole the Warren project received a good deal of criticism, even from those librarians who had experimented with computer systems and mechanization and were partly committed in this direction. The value of the book, coming at the present time, is for the light it throws on changing attitudes in the American approach to library automation and retrieval. While most authorities accept that some degree of mechanization is inevitable and must be provided for in planning new libraries there is a growing tendency to look for simpler and less expensive solutions to problems, to delay the search for total systems, and to question the once firmly-held view that conventional libraries are heading towards a breakdown. Unavoidably the British reader will unfavourably compare the Warren concept with our own satisfactorily-operating *National Lending Library for Science and Technology*.

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