Some general implicit processes for the numerical solution of differential equations

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Some general implicit processes are given for the solution of simultaneous first-order differential equations. These processes, which use successive substitution, are implicit analogues of the (explicit) Runge-Kutta processes. They require the solution in each time step of one or more sets of simultaneous linear equations, usually of a special and simple form.

Processes of any required order can be devised, and they can be made to have a wide margin of stability when applied to a linear problem.

Introduction

It is well known that problems of stability arise in the solution of parabolic partial differential equations. If the equation is linear, for example

\[ \frac{\partial x}{\partial t} = \kappa \frac{\partial^2 x}{\partial z^2} \]

and if it is replaced by a set of simultaneous ordinary differential equations

\[ \dot{x} = \phi(x) = Ax \]

then the solution is a sum of terms containing exponentials \( e^{-\kappa t} \). Any explicit numerical method of solving eqn. (2) (e.g. Runge-Kutta) replaces the exponentials by their truncated Taylor’s series during one time interval of the solution. The exponentials tend to zero as \( t \) becomes large, whereas the truncated Taylor’s series tend to infinity. A severe limitation on the length of the time intervals is thus introduced.

Crank and Nicholson (1947) pointed out that the restriction could be completely removed in linear problems by using the trapezoidal rule

\[ k_r = h_r \left\{ \frac{1}{2} \phi_{r-1} + \frac{1}{2} \phi_r \} \]

\[ x'_r = x_{r-1} + k_r \]

where \( h_r \) is the length of the \( r \)th time step, and the dash distinguishes the numerical from the exact solution of eqn. 2. This process replaces the exponentials occurring in the solution of eqn. (2) by the approximation

\[ \phi_r(t) = \frac{1 - \frac{1}{2} k_r t}{1 + \frac{1}{2} k_r t} \]

for which the equivalent of eqn. (5) is

\[ \phi_r(t) = \frac{1}{1 + k_r t} \]

This tends to zero as \( t \to \infty \).

Unfortunately, the process just described has a truncation error \( O(h^2) \), which makes it unsuitable when accurate solutions are needed. What has been said, however, leads naturally to the following question: are there alternative processes which have as good a truncation error as Crank and Nicholson’s, or better, and which at the same time have a margin of stability when applied to a difficult linear problem? If so we may expect these processes to remain stable in non-linear problems, and to allow the use of long time-steps with good accuracy.

A general implicit process

When the functions \( \phi \) are non-linear, implicit equations such as eqn. (3) can in general be solved only by iteration. This is a severe drawback, as it adds to the problem of stability, that of convergence of the iterative process. An alternative to eqn. (3), which avoids this difficulty, is

\[ (k_r)_r = h_r \left( \phi_r(t)_{r-1} + \frac{1}{2} \sum_j \left( \frac{\partial \phi_j}{\partial x_j} \right)_{r-1} (k_j)_r \right) \]

This set of linear equations can be solved directly for \( k_r \), and if each \( \phi_j \) depends on only a few of the \( x \) the solution can be carried out rapidly and easily.

A generalized implicit process may be obtained from eqn. (9) by analogy with Kopal’s treatment of the Runge-Kutta processes (Kopal, 1955). Let

\[ A(x) = A_0(x) = \left( \frac{\partial \phi(x)}{\partial x} \right) \]

and write

\[ k_r = h_r \left( \phi(x_{t-1}) + a_1 A(x_{t-1}) k \right) \]

\[ m_r = h_r \left( \phi(x_{t-1}) + a_2 A(x_{t-1}) + c_k m_0 \right) \]

\[ \ldots \]

\[ x_{t+1} = x_{t-1} + R_1 k_0 + R_2 L_0 + R_3 m_0 + \ldots \]
Solutions of differential equations

Then eqns. (11), (12), (13), etc., are linear implicit equations which may be solved successively to give $k_r, l_r, m_r$, etc. We shall say that such a process has $q$ stages if $R_q$ is not zero, but all preceding $R$ are zero.

By a straightforward but tedious calculation it is possible to expand $x_r - x_{r-1}$ 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:

$$h_r^2: \quad R_1 a_1 + R_2 (a_2 + b_1) = \frac{1}{2}$$  \hspace{1cm} (15)

$$h_r^3: \quad \begin{cases} R_1 a_1^2 + R_2[a_2^2 + (a_1 + a_2)b_1] = \frac{1}{6} \\ R_2(a_2c_1 + \frac{1}{2}b_1^2) = \frac{1}{6} \end{cases}$$  \hspace{1cm} (16)

$$h_r^4: \quad \begin{cases} R_1 a_1^3 + R_2[a_2^3 + (a_1^2 + a_1a_2 + a_2^2)b_1] = \frac{1}{24} \\ R_2(a_2c_1 + \frac{1}{2}b_1^2) = \frac{1}{24} \\ R_3(a_2c_1 + a_2c_1 + a_2b_1c_1 + a_2b_1^2) = \frac{1}{24} \\ R_2(\frac{1}{2}a_2c_1^2 + \frac{1}{2}b_1^3) = \frac{1}{24} \end{cases}$$  \hspace{1cm} (17)

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 $O(h^4)$. Two further conditions may then be applied.

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

$$a_1 = 1 + \sqrt[6]{6} = 1 - 2\sqrt{6} = 2.48286$$  \hspace{1cm} (20)

$$a_2 = 1 + \sqrt[6]{6} - 0.59175$$  \hspace{1cm} (21)

$$b_1 = c_1 = \left\{ -6 - \sqrt[6]{6} + \sqrt[6]{58 + 20\sqrt{6}} \right\} / (6 + 2\sqrt[6]{6})$$  \hspace{1cm} (22)

$$R_1 = 0.173876$$  \hspace{1cm} (23)

$$R_2 = 1.413154$$  \hspace{1cm} (24)

$$k_r = \frac{1}{h_r}\phi(x_r, y_r) + a_1 A(x_r, y_r) k_r$$  \hspace{1cm} (25)

$$x_r = x_{r-1} + h_r k_r$$  \hspace{1cm} (26)

$$y_r = y_{r-1} + \frac{h_r}{2} R_1 k_r$$  \hspace{1cm} (27)

The function corresponding to eqn. (5) is

$$\psi(t) = \frac{1 + k_r t - \frac{1}{3}(k_r t)^2}{1 + 2k_r t - \frac{1}{3}(k_r t)^2}$$  \hspace{1cm} (28)

which tends to $-0.8$ as $t \to \infty$. It can be shown that there is no two-stage process with truncation error $O(h^4)$ for which $\psi_0(t) \to 0$ 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 $\psi_0(t) \to 0$ as $t \to \infty$, provided that a truncation error $O(h^3)$ is acceptable. An example is obtained with

$$a_1 = a_2 = 1 - \sqrt[6]{2}/2, b_1 = (\sqrt[6]{2} - 1)/2.$$  \hspace{1cm} (29)

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

$$k_r = h_r\phi(x_r, y_r) + a_1 A(x_r, y_r) k_r$$  \hspace{1cm} (30)

$$x_r = x_{r-1} + h_r R_1 k_r$$  \hspace{1cm} (31)

with

$$a_1 = \frac{1}{2}(1 + i), R_1 = 1.$$  \hspace{1cm} (32)

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

$$\psi(t) = \frac{1}{1 + k_r t + \frac{1}{3}(k_r t)^2}$$  \hspace{1cm} (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


Book Review


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...