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A Taylor series method for numerical fluid mechanics

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SUMMARY. A method is proposed for the numerical solution of a large class of initial value problems in fluid mechanics. The method is shown to be non-dispersive, non-diffusive, and for equations with constant coefficients it is shown to be unconditionally stable, and indeed exact. For systems which contain only first-order derivatives, the method leads to "interpolation-only" solution techniques, obviating the need for numerical approximation of derivatives. Where coefficients in the equations are not constant, the scheme is of relatively low accuracy in the time-stepping. However, a systematic procedure is developed for generating schemes of high accuracy.

1. Introduction

The dominant feature of most fluid mechanics problems is that the fluid is flowing – an obvious fact, but which has often been neglected in numerical fluid mechanics. The Eulerian view of the fluid motion, and its differential equation description, has been carried over into the numerical solution of those equations. In most cases, with the spectacular exception of the method of characteristics and the less-successful technique of upwinding, no attention has been given to the flowing or convective nature of the solutions which are to be obtained. One could assert that because of this, the achievements of numerical fluid mechanics remain small in comparison with what they might have been; one has only to read an introduction to the subject, such as Noye (1978), Roache (1972) or Peyret & Taylor (1983), to be impressed by how most methods have decidedly unpleasant limitations. Some of the most obvious methods are unconditionally unstable. Some have exceptionally demanding stability limitations. It might be imagined that the most demanding problems would be those where diffusive and dispersive effects are small. That is not the case - the situation which obtains is that convection-dominated flows (where little change occurs) are considered to be the most difficult cases for computation! Some "upwinding" methods have tried to incorporate the convective nature of the flows, but most of these have severe problems with artificial diffusion. The plethora of recipes and methods is truly remarkable (see Leonard (1979) for an interesting and creative discussion of the problem).

In this paper an attempt is made to foster a new method for initial value problems in numerical fluid mechanics, through the use of high-order Taylor series solutions. By means of the partial differential equations, the operation of time differentiation is replaced by spatial differentiation, giving differential operators of infinite order. A general method is suggested which approximates the operators as if they had constant coefficients. This results in the generation of a single numerical scheme which can be used for a wide variety of problems, something of a rarity in numerical fluid mechanics. The scheme is independent of the method of spatial approximation, which is left as a different part of the problem, but one which is crucial to the application of the method.

2. The basic method - scalar version

In this section the case is considered where there is a single dependent variable, a single space variable, and where the time derivative is of first order only. This is the simplest case to be considered in this

paper. It includes several well-known equations from fluid mechanics.

Consider the partial differential equation for a scalar quantity $u(x,t)$, where x is position and t is time:

$$\frac{\partial u}{\partial t} = \underbrace{a_0(u,x,t)}_{\text{(source/sink)}} + \underbrace{a_1(u,x,t)\frac{\partial u}{\partial x}}_{\text{(convection)}} + \underbrace{a_2(u,x,t)\frac{\partial^2 u}{\partial x^2}}_{\text{(diffusion)}} + \underbrace{a_3(u,x,t)\frac{\partial^3 u}{\partial x^3}}_{\text{(dispersion)}} + \ldots \tag{1}$$

where, as shown, each of the a_i may be a function of u and the independent variables. Equations of this type come from a wide variety of applications in fluid mechanics, and include the following equations: convection, kinematic wave, diffusion, convective diffusion, Burgers, nonlinear Schrödinger, and the Korteweg-de Vries equations. The possible presence of nonlinearities and some of these high-order derivatives has made this family a rich area for mathematics. Of more interest in the present context, they have provided a stimulus and demanding testing ground for the development of techniques of numerical fluid mechanics.

The first step is to write (1) as

$$\frac{\partial u}{\partial t} = L(u,x,t,\partial/\partial x)\, u = Lu, \tag{2}$$

where L is the differential operator

$$L = a_0(u,x,t) + a_1(u,x,t)\frac{\partial}{\partial x} + a_2(u,x,t)\frac{\partial^2}{\partial x^2} + a_3(u,x,t)\frac{\partial^3}{\partial x^3} + \ldots.$$

In most problems, a set of initial conditions $u(x,0)$ is known and it is required to obtain the solution $u(x,t)$ by advancing in time numerically, possibly subject to boundary conditions on u for some values of x. This is usually done by solving the problem for a number of small increments in time Δ. The exact solution to the problem at a later time $t+\Delta$ at points in the interior can be written as the Taylor series

$$u(x,t+\Delta) = u(x,t) + \Delta\frac{\partial u}{\partial t}(x,t) + \frac{\Delta^2}{2!}\frac{\partial^2 u}{\partial t^2} + \ldots. \tag{3}$$

From (2) it is clear that differentiating with respect to time has the same effect as the application of L. The partial differential equation can be substituted for $\partial u/\partial t$, and this can be further differentiated to give

$$u_{tt} = L_t u + (Lu)(L_u)u + LLu, \tag{4}$$

where subscripts denote partial differentiation. Each of these terms now involve spatial differentiation only. The process can be repeated for higher orders, but it is clear that further differentiation will quickly give rather complicated expressions.

At this stage the first approximation is made, that at second and higher orders the dependence of L itself on the variables u, x, and t is neglected. Thus, (4) is approximated by $u_{tt} \approx L^2 u$, and it is simply shown that to all higher orders, $u_{ttt} \approx L^3 u$, and so on. In these expressions and subsequently in this work, L^n is interpreted as being the binomial expansion of L to the nth power such that the derivatives do not operate on any part of L itself. This will be referred to as the "constant-coefficient" approximation, which is exact if the quantities a_i in L are constant.

Substituting into the Taylor series (3) gives

$$u(x,t+\Delta) = u(x,t) + \Delta L u(x,t) + \frac{\Delta^2}{2!}L^2 u(x,t) + ... + O\left(\Delta^2\right). \tag{5}$$

Now, the usual shorthand is adopted, and (5) is written as

$$u(x,t+\Delta) = \exp(\Delta L)\, u(x,t) + O\left(\Delta^2\right), \tag{6}$$

If the spatial derivatives can be obtained this gives an explicit method of solution, While it may be thought that it is inconsistent to include terms of infinite order and to neglect some terms of second order in the constant coefficient approximation, it will he seen that the scheme (6) includes the most important

features of the solution, neglected by many numerical methods.

As an example, consider the one-dimensional convection equation $\partial u/\partial t + c\partial u/\partial x = 0$. In this case, $L = -c\partial/\partial x$, where c is a constant velocity convecting the passive scalar u. Scheme (6) becomes $u(x, t + \Delta) = \exp(-c\Delta\partial/\partial x)\, u(x, t)$, and we can consider the exponential operator to be the simple shift operator to give the scheme $u(x, t + \Delta) = u(x - c\Delta, t)$. In fact, this is the exact solution. This compares with a naive first-order finite-difference approach which might wish to approximate the partial differential equation by

$$\frac{u(x, t+\boldsymbol{\Delta}) - u(x, t)}{\Delta} \approx -c\frac{u(x + \delta, t) - u(x - \delta, t)}{2\delta},$$

to give a formula for $u(x, t + \Delta)$. This scheme is unconditionally unstable! A discussion of the application of the Taylor scheme and various other methods to the convection equation has been given by Fenton (1982).

3. Spatial approximation

To implement the Taylor scheme (6) it is necessary to evaluate the quantity $\exp(\Delta L)\, u(x, t)$. As this is a differentiation of infinite order, it might be expected that the computational difficulties would be rather formidable. Various approximations can be made, however, depending on the manner in which the dependence of u on x is approximated. For the case of Fourier series, no approximation is necessary, and some interesting interpretations of the nature of the method and its solutions can be made.

3.1 Finite Fourier Series

The infinitely-continuous nature of Fourier series, their analytical simplicity, and the use of fast methods for their evaluation all strongly suggest that they are particularly suitable. Let $u(x, t)$ be approximated by the finite Fourier series

$$u(x, t) = \sum_{j=-N/2}^{N/2}{}'' U_j(t)\, \exp\left(\mathrm{i}jkx\right), \tag{7}$$

where the Σ'' means that the contributions at the end points $j = \pm N/2$ are multiplied by half. In this series, $\mathrm{i} = \sqrt{-1}$ and k is the wavenumber $2\pi/\lambda$, where λ is the length of the computational domain. The use of the Fourier series implies that the function is continued periodically outside the domain of interest. This can lead to discontinuities at the ends, with resultant Gibbs phenomenon, but will not be discussed here.

For computational purposes the Fourier coefficients can be found by the (inverse) Fourier transform of the N equispaced values of u, $u_m = u(x_m, t) = u(m\lambda/N, t)$, $m = -N/2, .., N/2$. That is,

$$U_j(t) = \frac{1}{N} \sum_{m=-N/2}^{N/2}{}'' u_m(t)\, W^{-mj},$$

for $j = -N/2, \ldots, +N/2$, where $W = \exp(\mathrm{i}2\pi/N)$. These can of course be most conveniently found by a fast Fourier transform (FFT).

Substituting (7) into (6), and proceeding formally, interchanging the order of differential operation and summation, the following expression is obtained (the details of the summation in j are the same as for (7)):

$$u(x, t + \Delta) = \sum_{j}{}'' U_j(t) \exp\left(\Delta L(u, x, t, \partial/\partial x)\right)\, \exp(\mathrm{i}jkx) + O\left(\Delta^2\right).$$

If the exponential operator is now expanded, the differentiation performed, and the results regrouped as

an exponential function, the result is obtained:

$$u(x,t+\Delta) = \sum\nolimits''_j U_j(t) \exp\left(\Delta L(u,x,t,\mathrm{i}jk)\right) \exp(\mathrm{i}jkx) + O\left(\Delta^2\right).$$

and it can be seen that the $\partial/\partial x$ in the exponential operator has been replaced, giving an exponential function in terms of $\mathrm{i}jk$. If the explicit form (1) is substituted, the terms can be re-arranged to give

$$u(x,t+\Delta) = e^{a_0\Delta} \sum\nolimits_j U_j(t) \exp \mathrm{i}jk\left[x + \Delta\left(a_1 - a_3 j^2 k^2\right)\right] \exp\left[-\Delta a_2 j^2 k^2\right] + O\left(\Delta^2\right). \quad (8)$$

In this analysis, no attention has been paid to questions of convergence of the Fourier series.

The role and name of each of the terms in the original partial differential equation (1) now becomes clearer. The source/sink term contributes an *exponential* growth or decay. The convective term $a_1 \partial u/\partial x$ has the effect of shifting the phase of the solution. Momentarily ignoring other effects, every phase in the wave moves such that the wave height or concentration value which was at $x + a_1\Delta$ at time t is at x at time $t+\Delta$, showing the essentially convective nature of the scheme, and how upwinding is incorporated. This would have been made clearer if it had been written for a flow velocity of c, such that $a_1 = -c$, so that the value at $(x, t+\Delta)$ is that which was previously upstream at $(x - c\Delta, t)$. The present general case is complicated by the presence of a dispersive term, by which the speed of the phases depends on their wavelength, so that the speed of each is actually $-\left(a_1 - a_3 j^2 k^2\right)$, precisely the value it should be. The scheme (8), unlike most numerical methods, shows no numerical diffusion for the constant coefficient case; the effect of the convective and dispersive terms is such as merely to change the phase of the imaginary exponent, to shift the solution in x. Finally, the nature of the diffusive term is obvious, for it acts so as to reduce the amplitude of Fourier coefficient by an exponential factor $\exp\left[-\Delta a_2 j^2 k^2\right]$. This is a familiar and exact result from Fourier's solution of the heat equation.

The use of the Fourier approximation makes stability analysis rather simple as the stability of Fourier components can be studied directly. However, linear stability with constant coefficients only can be examined here. By writing the left side of (8) as a Fourier series, the following difference equation in spectral space is obtained:

$$U_j(t+\Delta) = U_j(t)\, e^{a_0\Delta} \exp\left[\mathrm{i}jk\Delta\left(a_1 - a_3 j^2 k^2\right)\right] \exp\left[-\Delta a_2 j^2 k^2\right].$$

From this it can be seen that the constant coefficient case is solved exactly, for the modes grow or decay in accordance with the growth/decay term, and decay with the diffusive term, at the correct rate. There is no growth of parasitic solutions, and the magnitude of the term containing the convective and dispersive terms is unity; they do not contribute to instability.

Each of the above interpretations follows from the use of the *infinite* Taylor series approach. If any other low-level approximation had been used, the physical nature of the terms would not have been made so obvious, nor their effects on the numerical solution so precisely separated, nor would the unconditional stability have been found. Also, of course, for problems in which the coefficients are constant, the scheme (8) is an exact solution. This seems sufficient justification for the use of the constant coefficient approximation to infinite order.

It should be noted, however, that in the form of (8), it would not be possible to use FFT's to evaluate the Fourier series if either a_1, a_2, or a_3 were functions of u or x. This does not present a major obstacle to the use of the Taylor scheme, though. It would be possible to make power series expansions of the exponential functions and to truncate at a finite order, so that FFT's could be used.

3.2 Cubic Splines

Another form of approximation may be used which is relatively robust, continuous, and is simply implemented: piecewise polynomial approximation, in particular, cubic splines. For a description of the theory, plus useful Fortran programs, reference can be made to Conte & de Boor (1980). With the splines, local approximation between node points $(x_m, u(x_m,t))$ is by a cubic polynomial such that there is continuity of gradient and curvature across the node points. The approximation can be written $u(x,t) = P_3(x)$, where P_3 is a piecewise cubic function, all of whose coefficients are functions of time,

not shown explicitly here.

Although the cubic splines can give accurate results for first and second derivatives, they are not so accurate for third derivatives, and here their application to equations with dispersive terms is ruled out. The method (6) now gives

$$u(x,t+\Delta) = \exp\left(\Delta a_0 + \Delta a_1 \partial/\partial x + \Delta a_2 \partial^2/\partial x^2\right)\ P_3(x) + O\left(\Delta^2\right),$$

which, on separating the order of the operations, acceptable within the constant coefficient approximation, and interpreting the exponential term with a first derivative in the exponent as a shift operator, gives

$$\begin{aligned} u(x,t+\Delta) &= e^{\Delta a_0}\, e^{\Delta a_2 \partial^2/\partial x^2}\, P_3\left(x+\Delta a_1\right) + O\left(\Delta^2\right) \\ &= e^{\Delta a_0}\left[P_3\left(x+\Delta a_1\right) + \Delta a_2 P_3''\left(x+\Delta a_1\right)\right] + O\left(\Delta^2\right). \end{aligned}$$

The nature of this solution is that the diffusion is allowed to take place calculated to first order only from the second derivative, then the solution is convected by an amount given by the local velocity, and cubic interpolation used to find the actual function value.

Performing a stability analysis of this result in spectral space, the result is obtained that

$$\frac{U_j(t+\Delta)}{U_j(t)} = e^{\Delta a_0} \exp\left[\mathrm{i} j k \Delta a_1\right]\left(1 - \Delta a_2 j^2 k^2\right).$$

The difference between this and the expression obtained above, when considering the stability using Fourier approximation, is that the last term here is an approximation to $\exp\left[-\Delta a_2 j^2 k^2\right]$. Stability would require that the magnitude of this term be never greater than unity, which for the largest component present, $j = N/2$, gives the stability criterion $\Delta a_2/\delta^2 \leqslant 2/\pi^2$, where δ is the magnitude of the space step. This compares with the forward-time-centred-space finite difference approximation, which gives $\Delta a_2/\delta^2 \leqslant 1/2$, and the cell Reynolds number criterion of $a_1\delta/a_2 < 2$, (Peyret & Taylor (1983, p.40); Roache (1972, p.42)). It is the latter criterion which is most demanding for convection-dominated flows. If typical values are considered, Flow velocity $a_1 = 1$, diffusivity $a_2 = 0.01$, then the latter criteria require $\delta < 0.02$ and $\Delta < 0.02$, both requiring many time and space steps. Using splines, the present method gives a criterion $\Delta < 0.2\delta^2$, with no restriction on δ.

4. The basic method - vector and higher-order equations

4.1 Taylor Method

If the dependent variable is a vector function, or if a second or higher-order time derivative appears in the partial differential equation such that a substitution gives a system of equations with first-order time derivatives, then a procedure analogous to that of Section 2 can be followed.

Consider the partial differential equation

$$\mathbf{u}_t = \mathrm{A}\mathbf{u}$$

where u is an n-vector, the subscript denotes partial differentiation, and $\mathrm{A} = \mathrm{A}(\mathbf{u}, \mathbf{x}, t, \nabla)$ is an $n \times n$ matrix with some terms which are spatial derivative operators. The quantity $\mathbf{x}$ is the position vector, and ∇ is the vector partial differential operator. The equation is homogeneous; attention will he restricted here to such cases. Procedures similar to those used previously yield the scheme

$$\mathbf{u}(\mathbf{x}, t+\Delta) = \exp(\Delta \mathrm{A})\, \mathbf{u}(\mathbf{x}, t) + O\left(\Delta^2\right), \tag{9}$$

where it is understood that the exponential of the matrix has significance as its power series expansion. It is not necessary to evaluate that expansion if the matrix A is diagonalizable, that is if there exist matrices D and C such that $\mathrm{A} = \mathrm{CDC}^{-1}$, where D is a diagonal matrix whose only entries are the n eigenvalues of A, $\lambda_1, \ldots, \lambda_n$ assumed here to be distinct and C is the matrix whose columns are the eigenvectors of A, corresponding to the eigenvalues appearing in D.

As D is a diagonal matrix, it is simply shown that the exponential of the matrix is given by $\exp(\Delta \mathrm{A}) = \mathrm{C}\Lambda\mathrm{C}^{-1}$, where Λ is a diagonal matrix whose elements are $\exp(\Delta\lambda_i)$, $i = 1, .., n$. The scheme (9) then becomes

$$\mathbf{u}(\mathbf{x}, t + \Delta) = \left(\mathrm{C}\Lambda\mathrm{C}^{-1}\right) \mathbf{u}(\mathbf{x}, t) + O\left(\Delta^2\right) \tag{10}$$

4.2 Example of Application

Consider the Saint-Venant equations governing the flow with velocity $u(x,t)$ and depth $h(x,t)$ in a rectangular channel in the presence of gravity g:

$$h_t + (uh)_x = 0 \quad \text{and} \quad u_t + (u^2/2 + gh)_x = 0.$$

Thus, if $\mathbf{u} = (h, u)$, these equations can be written as

$$\mathbf{u}_t = -\mathrm{A}\mathbf{u}_x, \quad \text{where} \quad \mathrm{A} = \begin{bmatrix} u & h \\ g & u \end{bmatrix}.$$

In this example the $\partial/\partial x$ has been able to be factored out, so that this problem is notationally slightly different from the general method described above. The scheme becomes $\mathbf{u}(x, t+\Delta) = \exp(-\Delta \mathrm{A}\partial/\partial x)\, \mathbf{u}(x,t) + O\left(\Delta^2\right)$.

The eigenvalues of A are given by $(u - \lambda)^2 - gh = 0$, and if the substitution $c = \sqrt{gh}$ is made, then $\lambda = u \pm c$. Even though there has been no mention of the word "characteristic" yet, the formality of the Taylor approach seems to be preparing to exploit the fact that information is transmitted at velocities of $u \pm c$, very familiar from the solution of this problem by characteristics. Now, the eigenvectors are $(\pm c, g)$, so that the matrices become

$$\begin{aligned} \mathrm{D} &= \begin{bmatrix} u + c & h \\ g & u - c \end{bmatrix}, \ \mathrm{C} = \begin{bmatrix} c & -c \\ g & g \end{bmatrix}, \quad \mathrm{C}^{-1} = \frac{1}{2gc} \begin{bmatrix} g & c \\ -g & c \end{bmatrix}, \\ \Lambda &= \begin{bmatrix} \exp\left(-\Delta\left(u + c\right)\partial/\partial x\right) & 0 \\ 0 & \exp\left(-\Delta\left(u - c\right)\partial/\partial x\right) \end{bmatrix}. \end{aligned}$$

The scheme then becomes (10). Performing the matrix multiplications, with interpretation of the elements of Λ as shift operators gives the final scheme

$$h\left(x, t + \Delta\right) = \tfrac{1}{2}\left(h_+ + h_-\right) + \frac{c}{2g}\left(u_+ - u_-\right) + O\left(\Delta^2\right), \tag{11a}$$

$$u\left(x, t + \Delta\right) = \tfrac{1}{2}\left(u_+ + u_-\right) + \frac{g}{2c}\left(h_+ - h_-\right) + O\left(\Delta^2\right), \tag{11b}$$

in which $c = \sqrt{gh(x,t)}$, $h_+ = h(x - (u + c)\Delta, t)$, and $h_- = h(x - (u - c)\Delta, t)$ *etc*.

It should be pointed out that the Taylor method in this context has not revealed the existence of characteristics in their classical sense for this problem. However, by using the constant coefficient approximation, the travelling-wave nature of the solution has been incorporated, and in a sense the method is characteristic-based. The equations (11) are in fact an *interpolatory* approximation to the system of partial differential equations: it can be shown by Taylor expansions that they are consistent with the original equations. To advance the solution at any stage, it is necessary only to interpolate in x at a constant time level of t to obtain values of functions at the positions $x - (u \pm c)\Delta$. Cubic splines seem to be the most natural way of doing this, combining accuracy and convenience, and have been used in such a way by Fenton (1982) to solve the convection equation numerically.

It can be shown that the system (11) is linearly stable. These expressions would seem to have a number of advantages over conventional finite difference methods, explicit schemes of which have been described by Zoppou & O'Neill (1981) as "... uneconomic, inflexible and inferior..." . Implicit schemes on the other hand seem to be complicated, and usually a trade-off between numerical stability and numerical diffusion must be made. The real alternative is to use characteristics, but these seem to have disadvantages in practice, in that they are often complicated to implement, the numerical accuracy is often limited and rarely made explicit, information is not readily available at specified x and t, and trivial changes in

equations can complicate application substantially.

Perhaps the most interesting result which can be inferred here is that if any system of equations contains only first derivatives, then the numerical scheme using (10) will involve shift operators only, and hence interpolation only, and no differentiation is necessary. This may pave the way for some changes in the numerical solution of equations such as the tidal equations, which have to be solved in the presence of complicated geometry; discretisations other than the familiar clumsy rectangles could be simply implemented.

5. Higher-order schemes

The time-stepping schemes developed so far in this work are all of relatively low order, with truncation errors of second order in Δ if the coefficients vary. This is barely acceptable for many practical applications. In this section these schemes are used to develop a systematic means of generating higher-order multi-time-level schemes, theoretically without limit.

The basic scheme (10), which includes (6) as a special scalar *case,* can be written as

$$\mathbf{u}(\mathbf{x}, t+\Delta) = \mathrm{B}(\Delta)\,\mathbf{u}(\mathbf{x}, t) + \sum_{n=2}^{\infty} \mathbf{e}_n(x,t)\Delta^n, \tag{12}$$

where the matrix $\mathrm{B}(\Delta) = \mathrm{CAC}^{-1}$. The dependence of B on Δ has been indicated, it is also dependent on $\mathbf{u}$, $\mathbf{x}$ and t but this is not shown explicitly. In (12) the as-yet unknown error terms are shown as infinite power series with coefficients $\mathbf{e}_n(x,t)$. The quantity $\boldsymbol{\delta}(\Delta)$ can be defined by

$$\boldsymbol{\delta}(\Delta) = \mathbf{u}(\mathbf{x}, t+\Delta) - \mathrm{B}(\Delta)\,\mathbf{u}(\mathbf{x}, t).$$

If (12) is written, not just for the next time level $t+\Delta$, but also for $t-\Delta$, the previous time level, and for $t-2\Delta$ and so on, the infinite set of equations can he written

$$\begin{bmatrix} 1 & 1 & 1 & \dots \\ 1 & -1 & 1 & \dots \\ 4 & -8 & 16 & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix} \begin{bmatrix} \Delta^2\mathbf{e}_2 \\ \Delta^3\mathbf{e}_3 \\ \Delta^4\mathbf{e}_4 \\ \dots \end{bmatrix} = \begin{bmatrix} \boldsymbol{\delta}(\Delta) \\ \boldsymbol{\delta}(-\Delta) \\ \boldsymbol{\delta}(-2\Delta) \\ \dots \end{bmatrix}.$$

This can be used to generate time-stepping schemes of arbitrary order. For example, if the lowest level of approximation is considered, just the first element of the matrix can be taken, giving the result

$$\Delta^2\mathbf{e}_2 = \boldsymbol{\delta}(\Delta) = \mathbf{u}(\mathbf{x}, t+\Delta) - \mathrm{B}(\Delta)\,\mathbf{u}(\mathbf{x}, t) + O\left(\Delta^3\right),$$

and by allowing the errors to be of second order (that of the left side), the basic scheme (10) is obtained.

If the next higher level of accuracy is considered, the first 2×2 submatrix is considered and the necessary eliminations made to give

$$\Delta^3\mathbf{e}_3 = \tfrac{1}{2}\left(\boldsymbol{\delta}(\Delta) - \boldsymbol{\delta}(-\Delta)\right) + O\left(\Delta^4\right),$$

and neglecting the third order terms gives

$$\mathbf{u}(\mathbf{x}, t+\Delta) = \mathbf{u}(\mathbf{x}, t-\Delta) + \left(\mathrm{B}(\Delta) - \mathrm{B}(-\Delta)\right)\,\mathbf{u}(\mathbf{x}, t) + O\left(\Delta^3\right). \tag{13}$$

This is the *leap-frog* version of the Taylor scheme, with the familiar third-order errors of such schemes, but which here inherits all the desirable properties of its lower-order antecedents. It should be noted that the operators $B(\pm\Delta)$ acting on $\mathbf{u}(\mathbf{x}, t)$ will necessitate interpolation and differentiation in $\mathbf{x}$ at the time level t, but at the previous time level $t-\Delta$ the only information required is the value of the function at $\mathbf{x}$, the computational point under consideration. This holds true in higher level schemes for prior time levels as well.

As (13) is a three-time-level scheme, it requires two sets of *initial* conditions to start. This should not be a problem, as it would be possible to generate a set at a second time level from those at the first by using

the fundamental two-time-level scheme ((10) or (6)) with a smaller step.

6. References

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