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A New Finite-Difference Diffusion Scheme

J. M. HOBSON, N. WOOD, AND P. J. MASON

UK Meteorological Office, London Road, Bracknell, Berkshire, RG12 2SZ, United Kingdom

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A new second-order accurate, explicit diffusion scheme is presented and discussed. The scheme is derived as a weighted average of the conventional, forward-in-time, explicit diffusion scheme over one grid length and the same scheme, but over two grid lengths. Varying the weighting factors produces a family of schemes. For optimum use, a new scheme with the weighting factor dependent on the viscous stability number is proposed. It is slightly more computationally expensive than the conventional explicit scheme (typically by 25%) but is numerically stable at viscous stability numbers four times as large. Further, it is about 20% computationally less expensive than the fully implicit scheme even in the simplest one-dimensional model. This "three-level, locally implicit" scheme has been implemented in both a simple one-dimensional diffusion model and also in a complex three-dimensional large-eddy simulation model. It has been found to behave well and is profitable in both models.

1. INTRODUCTION

Diffusion is an important physical process in most practical fluid dynamical problems and needs to be accurately represented in any finite-difference model of such problems. A large variety of numerical finite-difference schemes have been devised to model diffusion. However, each appears to suffer from one of three shortcomings.

The first is that the requirement of numerical stability can place a severe restriction on the permitted time-step for schemes such as the conventional, forward-in-time, second-order accurate, explicit scheme. This is especially so in models of atmospheric boundary layer flow, due to a combination of the high vertical resolution required to resolve the large gradients in velocity and temperature fields, and the high values for the eddy viscosity that are encountered. The simple explicit scheme, which at first sight appears computationally cheap, is actually expensive because of the number of steps required to integrate to a particular time.

The second shortcoming is exhibited by the fully implicit scheme. This scheme, taken in isolation from other physical processes in a model, places no restriction on the time-step (other than that required to limit truncation errors). However, solutions of such a scheme require, in one dimension, the inversion of an $n \times n$ matrix at each time-step (where n is the number of grid points). In one dimension this is computationally expensive and if applied to multiple dimensions, there is a considerable cost both in computation time and complexity. So, although this scheme does not suffer the problem of having to take many small time-steps, each time-step it does take is computationally very expensive.

The third shortcoming is that schemes which appear to have the benefits of both the simple explicit methods (low computation time per step) and also of the implicit ones (large time-step), have in the past, only achieved this at some other cost. For example, the scheme described by DuFort and Frankel [2] is computationally inexpensive and places no restriction on the time-step, but the solution only converges to the correct answer as the time-step tends to zero. In practice, this can place as stringent a requirement on the time-step as that encountered with the simple explicit scheme.

We start by discussing in more detail, examples of schemes which exhibit each of the three types of shortcoming mentioned above, demonstrating these by using a simple model. We then discuss a new scheme and find that it, too, suffers from its own shortcomings. However, from that basis, a whole family of schemes is derived as a method of overcoming these problems and an optimum scheme is obtained. This is a simple second-order accurate explicit scheme, so it is relatively cheap computationally, but the time-step restriction required for numerical stability is relaxed by a factor of four, compared with the conventional second-order explicit scheme. The merits of this scheme are demonstrated in a simple model and also in a much more complex, practical model, for which further refinement of the scheme is required.

2. A REVIEW OF SOME DIFFUSION SCHEMES

A simple one-dimensional model was written to review some of the schemes and investigate further new ones. The model simulates the purely diffusive behaviour of a viscous fluid, between two parallel, infinite plates. The upper plate is a distance H above the lower. Both plates and the fluid between them are initially moving at constant velocity U_H,

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then the lower plate is instantaneously stopped. The model describes the subsequent behaviour of the fluid by solving the one-dimensional diffusion equation,

$$\frac{\partial U}{\partial t} = \frac{\partial}{\partial Z}\left(\nu \frac{\partial U}{\partial Z}\right) \tag{1}$$

where U is the horizontal velocity of the fluid, t is time, ν is the kinematic viscosity, and Z is the vertical height, $Z = 0$ corresponding to the height of the lower plate.

The imposed boundary conditions are that there is no slip at either the moving, or the stationary plate (i.e., $U = 0$ at $Z = 0$ and $U = U_H$ at $Z = H$). The initial conditions are $U = U_H$ for all Z, except at the lower boundary.

The model has points above the upper plate and below the lower plate in order to impose the boundary conditions. Points are separated by distance ΔZ which can vary with height. In order to simplify the discussion within this section, ν is held constant and the vertical grid spacing is fixed so that ΔZ is constant. The steady state solution for this problem is then given by $U = U_H Z/H$.

In this section we discuss three schemes that were mentioned in the introduction using the model described above:

• The most simple method is a forward-in-time, explicit scheme. In finite-difference form it is written as

$$\frac{U_k^{t+1} - U_k^{t-1}}{2\,\Delta t} = \frac{\nu}{\Delta Z}\left(\frac{U_{k+1}^{t-1} - U_k^{t-1}}{\Delta Z} - \frac{U_k^{t-1} - U_{k-1}^{t-1}}{\Delta Z}\right), \tag{2}$$

where U_k^t represents U on vertical level k at time t and similarly U_{k+1}^{t-1} represents U on level $k + 1$ at time $t - \Delta t$.

Here, U taken at $t - \Delta t$ is used to calculate U at $t + \Delta t$. A linear stability analysis (see Haltiner and Williams [1, pp. 123–126]) shows that this method is conditionally stable on $\Delta t \leq \mathrm{T}_d$, where $\mathrm{T}_d = \Delta Z^2/(4\nu)$. Figure 1 shows results from the simple one-dimensional model using this scheme with a time-step of 0.8 T_d. Profiles are given at times (a) $t = \frac{1}{4}\mathrm{T}_D$; (b) $t = \frac{1}{2}\mathrm{T}_D$; (c) $t = \mathrm{T}_D$, and (d) $t = 2\mathrm{T}_D$, where $\mathrm{T}_D = H^2/(4\nu)$. T_D has been chosen as an appropriate time-scale for diffusion over the domain depth H.

• The fully implicit scheme in finite-difference form is

$$\frac{U_k^{t+1} - U_k^{t-1}}{2\,\Delta t} = \frac{\nu}{\Delta Z}\left(\frac{U_{k+1}^{t+1} - U_k^{t+1}}{\Delta Z} - \frac{U_k^{t+1} - U_{k-1}^{t+1}}{\Delta Z}\right). \tag{3}$$

Here U_{k+1}^{t+1} and U_{k-1}^{t+1} are unknown and U_k^{t+1} is the quantity required from the calculation. If the equation is re-written for all levels in the model, a tri-diagonal $n \times n$ matrix equation, where n is the number of vertical levels in the model, can be written and solved. This is unconditionally stable but has a greater computational cost. In the simple one-dimensional model this scheme used about twice as much computation time per time-step as the forward-in-time explicit scheme. Figure 2 shows a U profile at $t = 2\mathrm{T}_D$ for a run with a time-step of $4\mathrm{T}_d$. It should be noted that in most models, diffusion is not the only process that dictates the maximum size of the time-step, so beyond a certain point (which will be the time-step imposed by the next most limiting process), eliminating the restriction from the diffusion scheme becomes irrelevant.

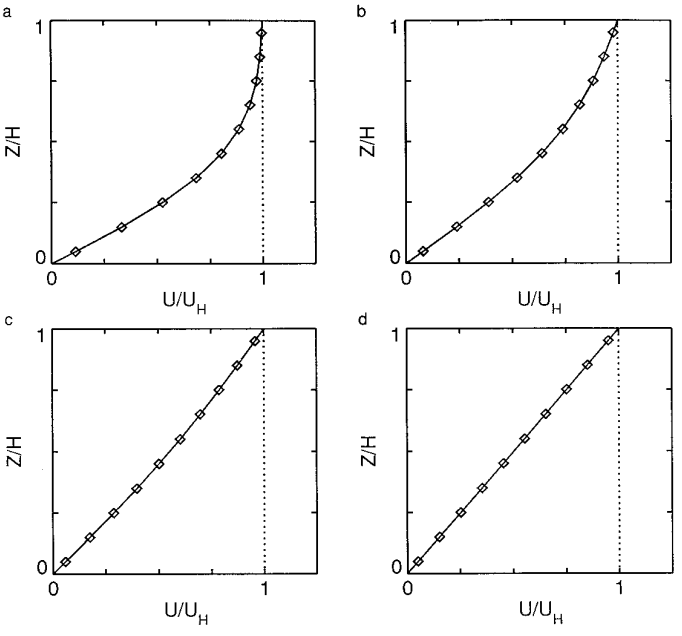

FIG. 1. Profiles of velocity, U, from a simple one-dimensional constant viscosity model using an explicit, forward-in-time diffusion scheme. The profiles shown are at times: (a) $t = \frac{1}{4}\mathrm{T}_D$; (b) $t = \frac{1}{2}\mathrm{T}_D$; (c) $t = \mathrm{T}_D$; and (d) $t = 2\mathrm{T}_D$. A time-step of $0.8\mathrm{T}_d$ was used in the run.

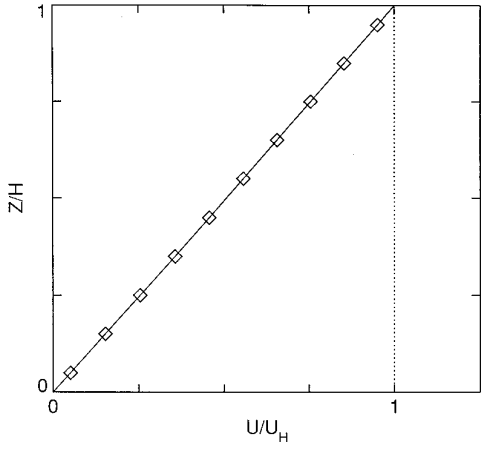

FIG. 2. The profile of velocity, U, from a simple one-dimensional constant viscosity model using the fully implicit diffusion scheme at time $t = 2\mathrm{T}_D$. A time-step of $4\mathrm{T}_d$ was used in the run.

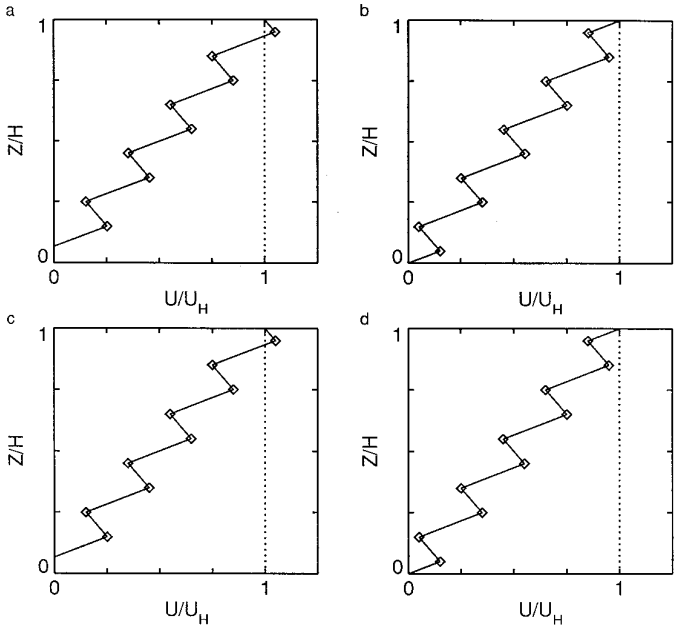

FIG. 3. Profiles of velocity, U, from a simple one-dimensional constant viscosity model using the DuFort–Frankel diffusion scheme. A time-step of $4T_d$ was used in the run. The profile at $t = 2T_D$ is shown in (a). The profile one time-step later is shown in (b). The profiles of the run 100 timesteps later than (a) and (b) are shown in (c) and (d), respectively.

• The method devised by DuFort and Frankel [2] can be written as

$$\frac{U_k^{t+1} - U_k^{t-1}}{2\,\Delta t} = \frac{\nu}{\Delta Z} \left(\frac{U_{k+1}^{t} - \tfrac{1}{2}(U_k^{t+1} + U_k^{t-1})}{\Delta Z} - \frac{\tfrac{1}{2}(U_k^{t+1} + U_k^{t-1}) - U_{k-1}^{t}}{\Delta Z} \right). \quad (4)$$

This is unconditionally stable, but it can produce spurious oscillatory modes. Figure 3a shows the U profile calculated using this scheme. A time-step of $4T_d$ has been used (the same as for the run with the implicit scheme) and the profile shows the run at $t = 2T_D$. Figure 3b shows the same run one time-step later. Figures 3c and 3d show the run 100 time-steps further on than 3a and 3b, respectively. Note that there are large oscillations about the mean profile, but that the scheme is stable (i.e., the oscillations are not growing). These oscillations are a well-known consequence of this scheme. As Dufort and Frankel [2], and then later Roache [3, pp. 61–64], note, as $\Delta t \to 0$ the scheme represented by Eq. (4) can be written as

$$\nu \left(\frac{\Delta t}{\Delta Z} \right)^2 \frac{\partial^2 U}{\partial t^2} + \frac{\partial U}{\partial t} = \nu \frac{\partial^2 U}{\partial Z^2}. \quad (5)$$

It is the presence of the first term on the left-hand side that allows the scheme to be unconditionally stable. Formally, the presence of this first term changes the equation from one of parabolic form to one of hyperbolic form. Hyperbolic equations can support waves which is evidenced in Fig. 3. Roache [3] also notes that, due to the presence of the first term on the left-hand side of Eq. (5), this scheme will converge to the correct solution and thereby eliminate spurious waves, only if $\Delta t \to 0$ more quickly than ΔZ. From Eq. (5) it can be seen that this limit can be interpreted approximately as requiring $\nu\,\Delta t/\Delta Z^2 \ll 1$. It is clear from Fig. 3 that, if $\nu\,\Delta t/\Delta Z^2 = 1$, waves are supported.

3. A NEW SCHEME

We now develop a new scheme which is an attempt to compromise between the forward-in-time explicit scheme and the fully implicit scheme without having the disadvantages of the DuFort–Frankel scheme. Any information takes a finite time to diffuse a certain distance. In the simple explicit diffusion scheme described by Eq. (2), any level, k, is only influenced in any one time-step by the $k + 1$ and $k - 1$ levels. This imposes a limitation on the time-step, such that Δt must be less than or equal to the time that any information takes to diffuse from one level to the next. By contrast, the fully implicit scheme allows any level, k, to be influenced by every other level each time-step and therefore, presents no limitation to the time-step. One might imagine that there is a middle ground between these methods, where the restriction on the time-step could be reduced without greatly affecting computation time. If, in the calculation for the kth level, a new scheme uses implicit values for terms at the $k + 1$ and $k - 1$ levels, but explicit values for terms at the $k + 2$ and $k - 2$ levels, this would allow information that is two levels away from the kth to have an influence on it and, hence, should allow the time-step limitation to be somewhat relaxed.

For each model level (in this case the kth), the following three equations can be written:

$$\frac{U_{k+1}^{t+1} - U_{k+1}^{t-1}}{2\,\Delta t} = \frac{\nu}{\Delta Z} \left(\frac{(U_{k+2}^{t-1} - U_{k+1}^{t+1})}{\Delta Z} - \frac{(U_{k+1}^{t+1} - U_k^{t+1})}{\Delta Z} \right) \quad (\mathscr{A}) \quad (6)$$

$$\frac{U_k^{t+1} - U_k^{t-1}}{2\,\Delta t} = \frac{\nu}{\Delta Z} \left(\frac{(U_{k+1}^{t+1} - U_k^{t+1})}{\Delta Z} - \frac{(U_k^{t+1} - U_{k-1}^{t+1})}{\Delta Z} \right) \quad (7)$$

$$\frac{U_{k-1}^{t+1} - U_{k-1}^{t-1}}{2\,\Delta t} = \frac{\nu}{\Delta Z} \left(\frac{(U_k^{t+1} - U_{k-1}^{t+1})}{\Delta Z} - \frac{(U_{k-1}^{t+1} - U_{k-2}^{t-1})}{\Delta Z} \right). \quad (\mathscr{B}) \quad (8)$$

We will refer to this general form of representation as the ''expanded'' form. As described above, the terms at $k +$

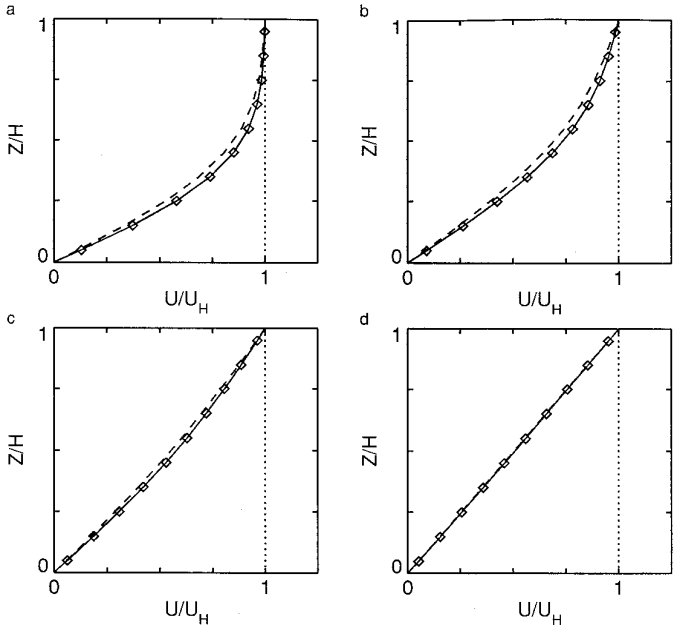

FIG. 4. Solid lines are profiles of velocity, U, from a simple one-dimensional constant viscosity model using the scheme represented by Eqs. (6)–(8). Dashed lines are the analytical solution to the same problem at the same model time. A time-step of T_d was used in the run. The profiles shown are at times (a) $t = \frac{1}{4}T_D$; (b) $t = \frac{1}{2}T_D$; (c) $t = T_D$; (d) $t = 2T_D$.

2 and $k - 2$ (labelled ($\mathscr{A}$) and ($\mathscr{B}$)) are evaluated at time $t - \Delta t$. All other terms are at time $t + \Delta t$. This set of three simultaneous equations has three unknowns, U_{k-1}^{t+1}, U_k^{t+1}, and U_{k+1}^{t+1}. However, we do not apply these equations simultaneously for all k, but are only interested locally in each level k and only solve for U_k^{t+1}. We then move to the $k + 1$ level and solve a similar set of equations for U_{k+1}^{t+1} and so on. The equations can be solved easily using, for example, a simple matrix method. Since they can be solved directly at each level, the scheme is an explicit one. It is a little more computationally expensive than the simple explicit method, but it is cheaper than the fully implicit scheme.

If the simple explicit scheme is conditionally stable on $\Delta t \le \Delta Z^2/(4\nu)$ then the physical arguments given above might suggest that the new scheme should be conditionally stable on $\Delta t \le (2\,\Delta Z)^2/(4\nu) = Z^2/\nu$. In fact, the stability analysis (see the Appendix) shows that it is unconditionally stable. The scheme, therefore, appears to give us something for nothing! Figure 4 shows U profiles, calculated using this scheme, from the simple one-dimensional linear model described in Section 2. Profiles are given at times (a) $t = \frac{1}{4}T_D$; (b) $t = \frac{1}{2}T_D$; (c) $t = T_D$; and (d) $t = 2T_D$. A time-step of T_d has been used in the run. The solid lines are results from the new scheme, the dashed are the analytical result (Batchelor [4, pp. 190–191]). Note that the curves are smooth with no oscillatory modes, but that the scheme appears to "run slow"; i.e., there is a time lag between the new scheme and the analytical solution it is trying to reproduce. This is not due to discretization errors as it does not occur for either forward-in-time explicit or fully implicit scheme with the same grid and time-step (i.e., in Figs. 1 and 2, the analytical solution lies exactly over the model profiles). The reason for the time lag is now investigated further and a solution to the problem is found.

Assuming constant ΔZ and ν the scheme can be rewritten in its explicit or "contracted" form as

$$(2C^2 + 4C + 1)\left(\frac{U_k^{t+1} - U_k^{t-1}}{2\,\Delta t}\right) = \nu\left(\underbrace{\frac{U_{k+1}^{t-1} - 2U_k^{t-1} + U_{k-1}^{t-1}}{\Delta Z^2}}_{(\mathscr{C})} + \underbrace{4C\frac{(U_{k+2}^{t-1} - 2U_k^{t-1} + U_{k-2}^{t-1})}{(2\,\Delta Z)^2}}_{(\mathscr{D})}\right), \tag{9}$$

where $C = 2\nu\Delta t/\Delta Z^2$.

The right-hand side of Eq. (9) can be divided into two halves. The first half, labelled ($\mathscr{C}$) is just the simple forward-in-time explicit scheme as shown in Eq. (2). The second half, labelled ($\mathscr{D}$) is the same scheme, but over two grid lengths, multiplied by a weighting factor. Symbolically, this approach can be represented by

$$\phi\frac{\partial U}{\partial t} = \chi\left[\frac{\partial U}{\partial t}\right]_{\Delta Z} + \psi\left[\frac{\partial U}{\partial t}\right]_{2\Delta Z}, \tag{10}$$

where $[\partial U/\partial t]_{\Delta Z}$ represents the explicit scheme over distance ΔZ and $[\partial U/\partial t]_{2\Delta Z}$ represents the explicit scheme over distance $2\Delta Z$. Physically, the usual explicit scheme works well for small values of C so that, as discussed above, information can only travel one grid space in one time-step. As C increases we require information from further away to influence U_k, so we would expect ψ to be proportional to C. For the above scheme

$$\chi = 1, \quad \psi = 4C, \quad \phi = 2C^2 + 4C + 1.$$

As the two terms on the right-hand side of Eq. (10) are complete diffusion schemes in their own right, we might expect that in order to get the correct amount of diffusion, we must impose $\chi + \psi = \phi$. Clearly this does not hold true with the above scheme, for which $\chi + \psi < \phi$, so this scheme models less diffusion than it should; hence, there is a time lag. This scheme exhibits the third type of shortcoming discussed in the Introduction, in that it is unconditionally stable, but it will only converge to the correct solution as $C \to 0$, so that $(2C^2 + 4C + 1) \to (4C + 1)$.

In order to avoid the problem of time lagging, we might suggest using values for χ, ψ, and ϕ of

$$\chi = 1, \quad \psi = 4C, \quad \phi = 4C + 1.$$

This leads to a diffusion scheme represented in the ''contracted'' form as

$$(4C+1)\left(\frac{U_k^{t+1} - U_k^{t-1}}{2\Delta t}\right) = \nu\left(\frac{U_{k+1}^{t-1} - 2U_k^{t-1} + U_{k-1}^{t-1}}{\Delta Z^2} + 4C\frac{(U_{k+2}^{t-1} - 2U_k^{t-1} + U_{k-2}^{t-1})}{(2\Delta Z)^2}\right). \tag{11}$$

It was found that the boundary conditions for this scheme, when implemented naively, put a much greater restriction on the time-step than the restriction from the scheme in the interior of the flow. In order to implement less restrictive boundary conditions it is necessary to write the scheme in the ''expanded'' form. The boundary conditions are then easy to implement (see Section 4 for further details of the implementation in the one-dimensional model).

It is straightforward to show that the above scheme shown in Eq. (11) is, in fact, equivalent to

$$\frac{U_{k+1}^{t+1} - U_{k+1}^{t-1}}{2\Delta t} = \frac{\nu}{\Delta Z}\left(\frac{(U_{k+2}^{t-1} - U_{k+1}^{t+1})}{\Delta Z} - \frac{(U_{k+1}^{t+1} - [2U_k^{t+1} - U_k^{t-1}])}{\Delta Z}\right) \tag{12}$$

$$\frac{U_k^{t+1} - U_k^{t-1}}{2\Delta t} = \frac{\nu}{\Delta Z}\left(\frac{(U_{k+1}^{t+1} - U_k^{t+1})}{\Delta Z} - \frac{(U_k^{t+1} - U_{k-1}^{t+1})}{\Delta Z}\right) \tag{13}$$

$$\frac{U_{k-1}^{t+1} - U_{k-1}^{t-1}}{2\Delta t} = \frac{\nu}{\Delta Z}\left(\frac{([2U_k^{t+1} - U_k^{t-1}] - U_{k-1}^{t+1})}{\Delta Z} - \frac{(U_{k-1}^{t+1} - U_{k-2}^{t-1})}{\Delta Z}\right). \tag{14}$$

When this scheme was coded into the simple linear one-dimensional model it did not exhibit any time lag.

Equations (12)–(14) have a curious form. The terms on the kth level in Eqs. (12) and (14) are a weighted average between the $(t + \Delta t)$ and $(t - \Delta t)$ time levels similar to the U_k terms that appear in the DuFort–Frankel scheme (see Eq. (4)). If we extend the same concept to the terms on the $(k + 1)$th and $(k - 1)$th levels and average them in the same way then we can write a more general form of the equations:

$$\frac{U_{k+1}^{t+1} - U_{k+1}^{t-1}}{2\Delta t} = \frac{\nu}{\Delta Z}\left(\frac{U_{k+2}^{t-1} - [(1-\alpha)U_{k+1}^{t-1} + \alpha U_{k+1}^{t+1}]}{\Delta Z} - \frac{[(1-\alpha)U_{k+1}^{t-1} + \alpha U_{k+1}^{t+1}] - [\beta U_k^{t+1} + (1-\beta)U_k^{t-1}]}{\Delta Z}\right) \tag{15}$$

$$\frac{U_k^{t+1} - U_k^{t-1}}{2\Delta t} = \frac{\nu}{\Delta Z}\left(\frac{(U_{k+1}^{t+1} - U_k^{t+1})}{\Delta Z} - \frac{(U_k^{t+1} - U_{k-1}^{t+1})}{\Delta Z}\right) \tag{16}$$

$$\frac{U_{k-1}^{t+1} - U_{k-1}^{t-1}}{2\Delta t} = \frac{\nu}{\Delta Z}\left(\frac{[\beta U_k^{t+1} + (1-\beta)U_k^{t-1}] - [(1-\alpha)U_{k-1}^{t-1} + \alpha U_{k-1}^{t+1}]}{\Delta Z} - \frac{[(1-\alpha)U_{k-1}^{t-1} + \alpha U_{k-1}^{t+1}] - U_{k-2}^{t-1}}{\Delta Z}\right). \tag{17}$$

When values of $\alpha = 1$ and $\beta = 2$ are used in the above equations, we regain the scheme represented by Eqs. (12)–(14). Similarly $\alpha = 1$ and $\beta = 1$ corresponds to the scheme represented by Eqs. (6)–(8). By changing the values of α and β we generate a whole family of diffusion schemes. Some of these schemes exhibit a time lag as described above and they all have different stability criteria. The optimum scheme of this type is the one which exhibits no time lag and is the most numerically stable. To obtain such a scheme, we start by deriving a relation between α and β to ensure no time lag.

We written in ''contracted'' form, the new family of schemes can be represented by

$$(1 + 2C(1+\alpha) + 2C^2(2\alpha - \beta))\left(\frac{U_k^{t+1} - U_k^{t-1}}{2\Delta t}\right) = \nu\left((1 - 2C(1-\alpha))\frac{(U_{k+1}^{t-1} - 2U_k^{t-1} + U_{k-1}^{t-1})}{\Delta Z^2} + 4C\frac{(U_{k+2}^{t-1} - 2U_k^{t-1} + U_{k-2}^{t-1})}{(2\Delta Z)^2}\right). \tag{18}$$

As before, this is a weighted average of a simple forward-in-time explicit scheme over one grid length and the same scheme over two grid lengths (See Eq. (10)). We found earlier, that when applying Eq. (10) we had to impose $\chi + \psi = \phi$ in order to give the correct amount of diffusion. If we impose a similar principle here, we obtain the equation

$$1 + 2C(1+\alpha) + 2C^2(2\alpha - \beta) = 1 + 2C(1+\alpha).$$

Hence, in order to give the correct amount of diffusion and avoid any time lag problems, we must limit our family of schemes to those for which

$$\beta = 2\alpha.$$

From this reduced family of schemes we now evaluate which is the most numerically stable (i.e., what values to use for α and β). The stability analysis of the general scheme results in the two following conditions (see the Appendix for details of this analysis):

$$C \leq \frac{3 + 3\alpha + \sqrt{16\alpha^2 - 24\alpha + 16 + 28\beta}}{2\alpha^2 - 12\alpha + 2 + 8\beta}, \quad C \leq \frac{1}{2(1-\alpha)}.$$

When $\beta = 2\alpha$ is imposed, the maximum value for C and, hence, the time-step can be found from the above conditions. This occurs when $\alpha = \frac{3}{4}$ and $\beta = \frac{3}{2}$. Thus, with these values, the scheme given by Eqs. (15)–(17) is optimal in that it exhibits no time lag and is stable provided $C \leq 2$ (i.e., $\Delta t \leq 4T_d$).

The scheme still uses implicitly derived values for the $k+1$, k, and $k-1$ levels and explicit values at $k-2$ and $k+2$. We shall, therefore, refer to this scheme as "the three-level, locally implicit" scheme. In this terminology the DuFort–Frankel scheme might be termed a "one-level, locally implicit scheme."

4. PROBLEMS ASSOCIATED WITH NON-UNIFORM GRIDS AND VARYING VISCOSITY

All the schemes and examples considered up to this point have only been concerned with simple laminar flow on a uniform grid. We now look at what happens to the scheme if we allow viscosity to vary both in time and space and, also, use a non-uniform, staggered grid. A representation of such a grid, with n vertical levels, is shown in Fig. 5. On this staggered grid the velocity U is stored at heights denoted by ZN and viscosity ν is stored at the alternate heights Z.

Writing

$$C_k^+ = \frac{2\Delta t\, \nu_k}{\Delta Z_k \Delta ZN_{k+1}}, \quad C_k = \frac{2\Delta t\, \nu_{k-1}}{\Delta Z_k \Delta ZN_k},$$

where k is any vertical level, Eqs. (15)–(17) can be rewritten for non-uniform staggered grid and varying viscosity as

$$\begin{aligned} U_{k+1}^{t+1} - U_{k+1}^{t-1} = {} & C_{k+1}^+(U_{k+2}^{t-1} - [(1-\alpha)U_{k+1}^{t-1} + \alpha U_{k+1}^{t+1}]) \\ & - C_{k+1}([(1-\alpha)U_{k+1}^{t-1} + \alpha U_{k+1}^{t+1}] \\ & - [\beta' U_k^{t+1} + (1-\beta')U_k^{t-1}]) \end{aligned} \tag{19}$$

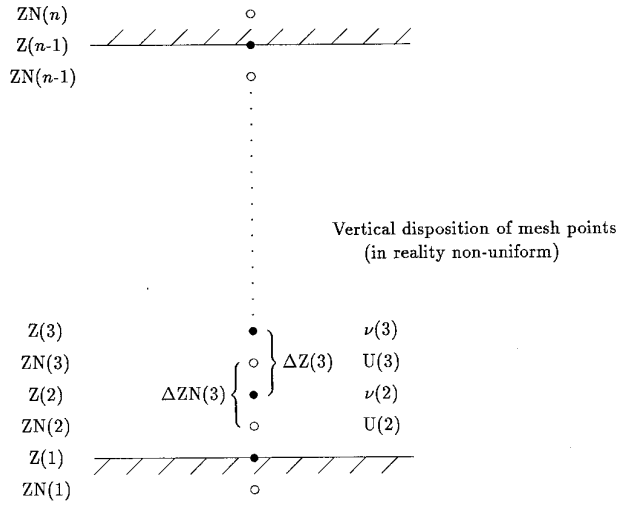

FIG. 5. The staggered vertical mesh used in the simple one-dimensional model. Note that in reality, the vertical disposition of grid points is non-uniform.

$$U_k^{t+1} - U_k^{t-1} = C_k^+(U_{k+1}^{t+1} - U_k^{t+1}) - C_k(U_k^{t+1} - U_{k-1}^{t+1}) \tag{20}$$

$$\begin{aligned} U_{k-1}^{t+1} - U_{k-1}^{t-1} = {} & C_{k-1}^+([\beta U_k^{t+1} + (1-\beta)U_k^{t-1}] \\ & - [(1-\alpha)U_{k-1}^{t-1} + \alpha U_{k-1}^{t+1}]) \\ & - C_{k-1}([(1-\alpha)U_{k-1}^{t-1} + \alpha U_{k-1}^{t+1}] \\ & - U_{k-2}^{t-1}). \end{aligned} \tag{21}$$

In the above equations, we have introduced β' and β. These are no longer equal to each other, as in the simple case. The introduction of β' was found necessary because when written in "contracted" form with $\beta' = \beta$, Eqs. (19)–(21) were found to exhibit a time lag. To determine the values of β' and β, we use the same procedure as described for the uniform case. A matrix equation is formed from the three equations. When it is solved and the criterion that we must have the correct amount of diffusion is imposed, we obtain the following expressions for β' and β in terms of α:

$$\beta' = \alpha\left(1 + \frac{C_{k+1}^+}{C_{k+1}}\right), \quad \beta = \alpha\left(1 + \frac{C_{k-1}}{C_{k-1}^+}\right).$$

These expressions can be substituted back into Eqs. (19) and (21), respectively, to provide us with a scheme that works, without a time-lag, for models with non-uniform staggered grid and varying viscosity, but reduces to Eqs. (15)–(17) for uniform grid spacing and constant viscosity. The value of α to be used with this scheme is taken from the linear stability analysis described above (i.e., $\alpha = \frac{3}{4}$). The complexity of the stability analysis for the scheme with

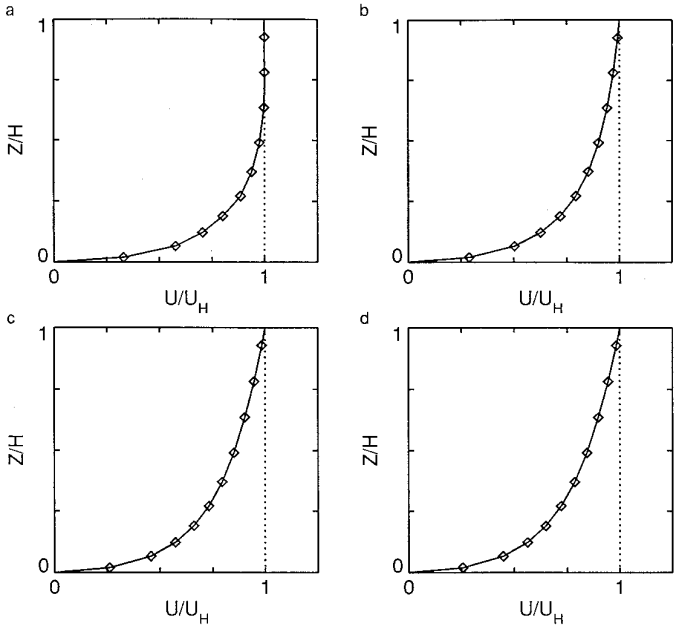

FIG. 6. Profiles of velocity, U, from a simple one-dimensional model with non-uniform, staggered vertical grid and varying viscosity. The "three-level, locally implicit" scheme was used for this run. The profiles shown are at times (a) $t = \frac{1}{4}T_D$; (b) $t = \frac{1}{2}T_D$; (c) $t = T_D$; (d) $t = 2T_D$.

non-uniform grid spacing and varying viscosity prevents a more general determination of α.

It is worth noting that the expressions for β' and β can be affected by the boundary and it may be necessary to re-evaluate them, although with the boundary conditions employed in the simple one-dimensional model it was not necessary. The boundary conditions were implemented for this model by re-writing Eqs. (19)–(21) with substituted values for the model variables at the boundaries. For example, the solution for U_k^{t+1} on the level $k = 2$ requires knowledge of U_1^{t+1}. This is given by the no-slip boundary condition at the lower, stationary plate (i.e., $U_1 = -U_2$). This condition is substituted into the last term of Eq. (20). Equation (19) remains unchanged by the boundary condition, but as U_1^{t+1} is known in terms of U_2^{t+1}, Eq. (21) is not required. Thus, at the level $k = 2$, Eqs. (19)–(21) reduce to

$$\begin{aligned} U_3^{t+1} - U_3^{t-1} = C_3^+(U_4^{t-1} - [(1-\alpha)U_3^{t-1} + \alpha U_3^{t+1})] \\ - C_3([(1-\alpha)U_3^{t-1} + \alpha U_3^{t+1}] \\ - [\beta' U_2^{t+1} + (1-\beta')U_2^{t-1}]) \end{aligned} \quad (22)$$

$$U_2^{t+1} - U_2^{t-1} = C_2^+(U_3^{t+1} - U_2^{t+1}) - C_2(2U_2^{t+1}). \quad (23)$$

These two simultaneous equations are then solved for U_2^{t+1}. This procedure is then repeated in a similar manner for all levels that are affected by the boundary conditions.

Figure 6 shows U profiles from the model using non-uniform grids and varying viscosity with the new "three-level, locally implicit" scheme. The profiles are shown at times: (a) $t = \frac{1}{4}T_D$; (b) $t = \frac{1}{2}T_D$; (c) $t = T_D$; and (d) $t = 2T_D$. As in Section 2, $T_D = H^2/(4\nu)$, but as viscosity is now a varying quantity, the value used for ν is its value at the height $H/2$ from the equilibrium state. A fixed time-step was used throughout the run. The value of the time-step was empirically chosen so that it remained just less than the minimum value of $\Delta Z^2/\nu$, both in space and time during the run.

TABLE I

Comparison of Computation Times from One-dimensional Model Runs with a Non-uniform, Staggered Grid and Varying Viscosity

Scheme	No. of vertical levels	No. of time-steps	Time[a] (s)	Normalized time[b]
Forward-in-time	10	1 000 000	30.7	1.00
Explicit scheme	100	100 000	27.0	1.00
	1 000	10 000	26.4	1.00
Fully implicit	10	1 000 000	47.0	1.53
scheme	100	100 000	43.9	1.63
	1 000	10 000	44.4	1.68
"Three-level, locally	10	1 000 000	38.4	1.25
implicit" scheme	100	100 000	34.1	1.26
	1 000	10 000	33.6	1.27

[a] Computation times for model runs on a DEC 3000 Model 400 Alpha Workstation.
[b] Computation times normalized by the time taken for the forward-in-time explicit run with the same number of levels.

All the various schemes discussed so far were run using this version of the model to give a comparison of the various computation times for the non-uniform case. The results are summarised in Table I.

The new explicit scheme was about 25% slower than the simple explicit scheme, but it can be run with a time-step which is four times the size of that used with the simple explicit scheme. The fully implicit scheme ran up to 68% slower than the simple explicit scheme. Although it can theoretically be run with any time-step, in reality, factors other than the diffusion scheme will limit the time-step. The extra complexity and added computation time, probably restricts the use of the implicit scheme to one-dimensional models.

5. USE OF THE SCHEME IN A MORE COMPLEX MODEL

Most practical applications require models that are more complicated than the simple ones discussed so far. First, the model may be three-dimensional, with diffusion in all directions and, second it is quite likely that it will be

modelling other processes as well as diffusion, such as advection, pressure gradient and for atmospheric models, Coriolis effects. When attempting to add the new scheme into the complex model, it quickly became apparent that it will not be efficient to represent all diffusion terms with the ''three-level, locally implicit'' scheme. The stability of all the diffusion terms is investigated in order to decide which terms to represent with the new scheme. The performance of the model with the new scheme is then tested.

Ignoring the extra terms due to advection etc., the three-dimensional diffusion equation for incompressible flow (for U only) becomes

$$\frac{\partial U}{\partial t} = \overbrace{\frac{\partial}{\partial x}\left(2\nu\frac{\partial U}{\partial x}\right)}^{(\mathscr{A})} + \frac{\partial}{\partial y}\left(\nu\left[\frac{\partial U}{\partial y} + \frac{\partial V}{\partial x}\right]\right) + \overbrace{\frac{\partial}{\partial z}\left(\nu\left[\frac{\partial U}{\partial z} + \frac{\partial W}{\partial x}\right]\right)}^{(\mathscr{B})}. \tag{24}$$

Coding all these terms into a scheme of the type described above would be extremely complicated. In particular, this scheme may not lend itself to coding the cross terms ($\mathscr{A}$) and ($\mathscr{B}$). The resulting code may take more computation time than it saves, although allowing a larger time-step. A comparison of the stability of each of the terms in the equation was performed in order to find which terms were most limiting to the stability and, hence, the time-step. In order to simplify the procedure, the viscosity is assumed constant. In reality, however, the viscosity has strong gradients which may affect the stability to some extent.

Term ($\mathscr{A}$) $(\partial/\partial y)(\partial V/\partial x)$ is analytically identical to $(\partial/\partial x)(\partial V/\partial y)$. It can be shown that this holds true even in finite-difference terms. Similarly term ($\mathscr{B}$) $(\partial/\partial z)(\partial W/\partial x)$ can be re-written as $(\partial/\partial x)(\partial W/\partial z)$. Equation (24) can then be re-written as

$$\frac{\partial U}{\partial t} = \overbrace{2\nu\left(\frac{\partial^2 U}{\partial x^2}\right)}^{(\mathscr{C})} + \overbrace{\nu\left(\frac{\partial^2 U}{\partial y^2}\right)}^{(\mathscr{D})} + \overbrace{\nu\left(\frac{\partial^2 U}{\partial z^2}\right)}^{(\mathscr{E})} + \overbrace{\nu\frac{\partial}{\partial x}\left(\frac{\partial V}{\partial y} + \frac{\partial W}{\partial z}\right)}^{(\mathscr{F})}. \tag{25}$$

The stability criterion for the explicit scheme currently used is that $\Delta t \leq \Delta^2/4\nu$, where Δ is a measure of the grid spacing. In many atmospheric applications Δx and Δy are much larger than Δz. Therefore, term ($\mathscr{D}$) is likely to be more stable when using the explicit scheme than term ($\mathscr{E}$). Invoking mass continuity, $\partial U/\partial x + \partial V/\partial y + \partial W/\partial z = 0$, term ($\mathscr{F}$) becomes $-\nu(\partial^2 U/\partial x^2)$. Adding ($\mathscr{C}$) to ($\mathscr{F}$) in this linear analysis, now gives us $\nu(\partial^2 U/\partial x^2)$, which is similar in stability terms to ($\mathscr{D}$). Term ($\mathscr{E}$), therefore is the most restrictive to stability, so this term is evaluated using the ''three-level, locally implicit'' scheme. All other terms are evaluated using the conventional forward-in-time explicit scheme.

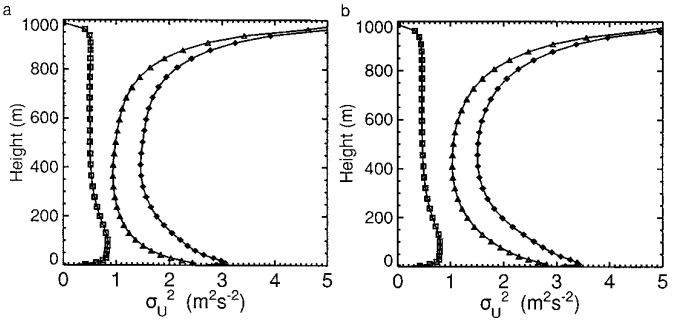

FIG. 7. Profiles of horizontal velocity variance, σ_u^2, from a run of a large-eddy model. Profiles from the run using the ''three-level, locally implicit'' scheme are shown in (a). The conventional explicit scheme was used to produce the profiles in (b). Squares mark the subgrid velocity variances, triangles, mark the resolved velocity variances, and diamonds mark the total.

The model used for the tests was the large-eddy model described by Mason [5]. In practice, when using this model, two processes limit the size of the time-step. There is a limit imposed by the diffusion scheme and another by the advection scheme. The time-step is chosen by the model to be as large as possible, given these constraints. In order to minimise the problem of having the time-step limited by the advection scheme, a simulation was chosen in which the mean horizontal flow velocities would remain very small. This simulation was initialised with small random velocity perturbations to a zero mean flow. A constant surface heat flux was imposed, leading to a simulation of free convective conditions. At the top boundary a stress-free rigid lid was imposed.

Figure 7 shows the horizontal velocity variance, σ_u^2, obtained by averaging over complete horizontal slices, then averaging these values over the previous 5000 s when the run had reached a time of 20,000 s. Tests indicate that these quantities have reached a statistical equilibrium. The profiles marked with squares show the parametrized (or subgrid) turbulence, triangles show the velocity variances resolved in the model and diamonds are the total velocity variances. Figure 7a shows profiles of σ_u^2 from a run that used the ''three-level, locally implicit'' scheme for the vertical diffusion terms. Figure 7b shows the same profiles from a run in which all the diffusion terms were evaluated using the conventional explicit scheme. Figure 8 shows the vertical velocity variance, σ_w^2 (which has been averaged in a similar way to σ_u^2). Figures 8a and 8b are profiles from runs using the different schemes as with Fig. 7. The profiles

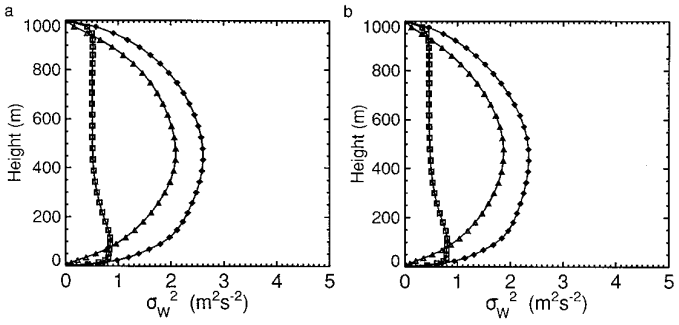

FIG. 8. Profiles of vertical velocity variance, σ_w^2, from a run of a large-eddy model. Profiles from the run using the ''three-level, locally implicit'' scheme are shown in (a). The conventional explicit scheme was used to produce the profiles in (b). Squares mark the subgrid velocity variances, triangles mark the resolved velocity variances, and diamonds mark the total.

are similar in general shape. Other diagnostics were reviewed and no significant differences were found. These results are not conclusive and further tests of the scheme are underway. Nevertheless, they do suggest the scheme is behaving well.

When using this model, the run with the new scheme ran 18% slower per time-step than the run using the forward-in-time explicit scheme, but the time-step was always at least twice the size. This meant that the simulation using the new scheme took just 50% of the time taken for the run using the forward-in-time explicit scheme.

6. CONCLUSIONS AND COMMENTS

We have identified and discussed examples of three types of diffusion scheme, each one displaying a different shortcoming. A family of new diffusion schemes has been proposed. Analysis of this family provides an understanding of the limitation of its various members and allows a new scheme to be derived as the optimum member of the family. This new scheme is an attempt to combine the computational simplicity of the conventional forward-in-time explicit scheme with the advantage of the larger time-step that can be gained from using the fully implicit scheme. Below, the optimum scheme is written in the form of a weighted average of the conventional forward-in-time explicit scheme over one grid length and the same scheme, but over two grid lengths,

$$\left(1+\frac{7C}{2}\right)\left(\frac{U_k^{t+1}-U_k^{t-1}}{2\Delta t}\right) = \nu\left(\left(1-\frac{C}{2}\right)\left(\frac{(U_{k+1}^{t-1}-2U_k^{t-1}+U_{k-1}^{t-1})}{\Delta Z^2}\right) + 4C\left(\frac{(U_{k+2}^{t-1}-2U_k^{t-1}+U_{k-2}^{t-1})}{(2\Delta Z)^2}\right)\right). \quad (26)$$

Here, grid spacing and viscosity are assumed constant. See Eqs. (19)–(21) for the more general form.

The scheme is second-order accurate and explicit in nature. The form of Eq. (26) (referred to as the ''contracted'' form) resembles the fourth-order accurate, centred explicit scheme (which for stability requires $C \leq \frac{3}{8}$). However, the weighting factors, rather than being constants as in the fourth-order scheme ($\chi = \frac{4}{3}$, $\psi = -\frac{1}{3}$, $\phi = 1$), are dependent on the viscous stability parameter, C. It is this that formally limits the scheme to be second-order accurate, but which permits the use of a relatively large time-step, as stability for this scheme requires $C \leq 2$.

Another way of writing the scheme has been given and referred to as the ''expanded'' form (see Eqs. (19)–(21)). It was from this form that the scheme was originally derived. When written in this way the scheme can be interpreted as being an intermediate between the conventional simple explicit scheme and the fully implicit scheme, in that all the terms contributing directly to a level (for example, k), are evaluated at time $t + \Delta t$ with a further equation being written for any unknown terms (i.e., U_{k+1}^{t+1} and U_{k-1}^{t+1}). Terms involving U_{k+2} and U_{k-2} are evaluated explicitly (i.e., at time $t - \Delta t$). As a result of this, the scheme is referred to as being ''three-level, locally implicit.''

The ''three-level, locally implicit'' scheme has been coded into a general one-dimensional model (with varying viscosity and non-uniform staggered grid) and also into a complex large-eddy simulation model. The scheme took 18% more computation time per time-step than the conventional explicit scheme in the latter model, but can, theoretically run with a time-step four times as large. In the test we ran, the time-step was, on average, over twice as large as the time-step used with the conventional explicit scheme. Other factors within the model restricted any further increase in the time-step. Even so, this represented a time saving of 50% over the entire run. In the one-dimensional model, the new scheme ran 20% faster than the fully implicit scheme. In order for the fully implicit scheme to be beneficial, the time-step would have to be increased to accommodate the additional computation time. But as we have already mentioned, the time-step had already reached the restriction of the next most limiting process, so the fully implicit scheme would only slow down the run.

In principle, the concept of the ''three-level, locally implicit'' scheme could be generalized to form an ''m-level locally implicit'' scheme. When $m = 1$ we have the scheme similar to the Dufort–Frankel scheme and when $m = n$ (where n is the number of grid points in the domain), we have the fully implicit scheme. However, we anticipate that for m intermediate between three and n, the complexity of the scheme, evaluation of boundary conditions and ensuring that the scheme does not exhibit any time lag would negate any benefit obtained by further relaxing the restriction on the time-step.

APPENDIX: STABILITY ANALYSIS FOR THE "THREE-LEVEL, LOCALLY IMPLICIT" SCHEME

Assuming constant grid spacing and viscosity, Eqs. (15), (16), and (17) reduce to

$$\begin{aligned} U_k^{t+1} = [&C^2(U_{k+2}^{t-1} + U_{k-2}^{t-1}) \\ &+ (C - 2C^2(1-\alpha))(U_{k+1}^{t-1} + U_{k-1}^{t-1}) \\ &+ (1 + 2C\alpha + 2C^2(1-\beta))U_k^{t-1}] \\ &/[1 + C(2 + 2\alpha) + C^2(4\alpha - 2\beta)] \end{aligned}$$

where $C = 2\nu\Delta t/\Delta Z^2$.

Following the von Neumann stability analysis procedure (see Roache [3, pp. 42–45]) we substitute a Fourier series expansion of the solution to the above equation, $U_k^t = A\lambda^{n\Delta t}e^{ikm\Delta Z}$, where $A\lambda^{n\Delta t}$ is the amplitude function of the time-level n of a particular component whose wave number is k. The displacement in time and vertical distance are denoted by the integers n and m, respectively. This substitution leads to

$$\begin{aligned} \lambda^2 = [&C^2(e^{2ik\Delta Z} \\ &+ e^{-2ik\Delta Z}) + (C - 2C^2(1-\alpha))(e^{ik\Delta Z} \\ &+ e^{-ik\Delta Z}) + (1 + 2C\alpha + 2C^2(1-\beta))] \\ &/[1 + C(2 + 2\alpha) + C^2(4\alpha - 2\beta)]. \end{aligned}$$

Re-writing and substituting $X = \cos(k\Delta Z)$ leads to

$$\begin{aligned} \lambda^2 = [&4C^2X^2 + 2(C - 2C^2(1-\alpha))X + 1 \\ &+ 2C\alpha + 2C^2(1-\beta) - 2C^2] \\ &/[1 + C(2 + 2\alpha) + C^2(4\alpha - 2\beta)]. \end{aligned}$$

Stability requires $-1 \le \lambda^2 \le 1$.

Taking the left-hand-side of the inequality leads to

$$0 \le (4\alpha - 4\beta - (1-\alpha)^2)C^2 + (3 + 3\alpha)C + \tfrac{7}{4}.$$

Factorizing the quadratic equation and eliminating one of the terms, as it is always positive, gives the requirement

$$C \le \frac{3 + 3\alpha + \sqrt{16\alpha^2 - 24\alpha + 16 + 28\beta}}{2\alpha^2 - 12\alpha + 2 + 8\beta}.$$

The right-hand side of the inequality leads to

$$C \le \frac{1}{2(1-\alpha)}.$$

In the case of $\alpha = 1$, $\beta = 1$ (appropriate to the scheme given by Eqs. (6)–(8)) both the above inequalities are satisfied for all C. Hence this scheme, although it exhibits a time lag, is unconditionally stable.

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