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Stable Schemes for Partial Differential Equations: The One-Dimensional Diffusion Equation

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Non-linear diffusion equations with numerical stability problems are common in many branches of science. An example is the k-diffusion parametrization for vertical turbulent mixing in atmospheric models that creates a system of non-linear diffusion equations with stability problems. In this paper a new algorithm to solve the one-dimensional diffusion equation is presented. This method, which is stable by design, is quite general and can be used in other partial differential equations. Results with the new scheme compare well with analytical solutions, and a study with a system of two non-linear diffusion equations shows that the new method is more stable than more traditional schemes. © 1999 Academic Press

Key Words: diffusion equation; numerical stability; non-linear diffusion.

1. INTRODUCTION

In atmospheric models vertical turbulent mixing is usually parametrized using a k-diffusion approach, where k depends on the mean variables. This parametrization creates a system of non-linear diffusion equations with numerical stability problems [1, 2]. This type of problem is one of the reasons the time step of climate models cannot be significantly increased [13]. Non-linear diffusion equations are used to model a variety of different phenomena, from engineering flows [5] and magnetohydrodynamics [6] to insect dispersal [4]. These models suffer from similar types of numerical stability problems, and a method that “solves” these problems in a very general way would have a wide range of applicability.

The equation for the atmospheric turbulent diffusion of a variable A can be solved with an implicit scheme, and a stability analysis shows that this scheme is unconditionally stable for the simple case of a constant k. However, k is not constant (neither in space nor in time) and usually is a non-linear function of the mean variables. In practice, the problem is often solved with an implicit formulation for A and an explicit formulation for k, but such

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a scheme is not necessarily stable in all circumstances [1]. Due to the stability problem a scheme usually referred to as "more-than-implicit" or "over-implicit", which corresponds to an implicitness factor larger than 1 [1], has been used in atmospheric models [2, 3]. This problem is particularly relevant in atmospheric models, such as climate and numerical weather prediction models, where a system of several non-linear diffusion equations has to be solved in a given fixed vertical grid.

The aim of this paper is to present a new type of algorithm with which to solve the one-dimensional diffusion equation. This method is, in principle, stable by design for any value of the stability coefficient. In Section 2 the new scheme is described. A derivation of the diffusion equation is presented in Section 3 in order to show an analogy with the new scheme. A discussion of some properties of the scheme is presented in Section 4. In Subsection 5.1 the results of simple tests are shown. Although this work is mainly concerned with the constant diffusion coefficient case, in Subsection 5.2, a situation that involves a variable k is studied in order to illustrate the potential advantages of the new method in dealing with non-linear diffusion equations. Some conclusions are presented in Section 6.

2. THE SCHEME

2.1. *The Explicit Method*

The one-dimensional diffusion equation for a generic property A is

$$\frac{\partial A}{\partial t} = \frac{\partial}{\partial x}\left(k\frac{\partial A}{\partial x}\right). \tag{1}$$

Discretizing the one-dimensional diffusion equation in space and explicitly in time (assuming grid spacing is uniform and the diffusion coefficient k is constant) gives

$$A_j^{n+\Delta t} = A_j^n + k\frac{\Delta t}{\Delta x^2}\left(A_{j+\Delta x}^n - 2A_j^n + A_{j-\Delta x}^n\right), \tag{2}$$

where Δt is the time step, Δx is the grid length, n is the time discretization index, and j is the space discretization index. The stability coefficient is

$$\alpha = k\frac{\Delta t}{\Delta x^2}. \tag{3}$$

A simple stability analysis shows that if $\alpha \leq 0.5$, Eq. (2) is stable and if $\alpha > 0.5$ the equation is unstable.

2.2. *The New Scheme*

The discretized version of the one-dimensional diffusion equation for the new scheme proposed here can be written as

$$A_j^{n+\Delta t} = A_j^n + k\frac{\Delta t}{\Delta s^2}\left(A_{j+\Delta s}^n - 2A_j^n + A_{j-\Delta s}^n\right). \tag{4}$$

To obtain Eq. (4) the spatial partial derivative is approximated by a finite difference along the distance Δs, which does not have to be equal to the grid length and which can be determined by imposing a fixed stability number $\beta \leq \frac{1}{2}$:

$$k\frac{\Delta t}{\Delta s^2} = \beta \qquad \Leftrightarrow \qquad \Delta s = \pm\sqrt{k\Delta t/\beta}. \tag{5}$$

The values of A at the rhs of Eq. (4) can then be obtained by interpolation from the original grid. For a stability coefficient of $\frac{1}{2}$ this is

$$k\frac{\Delta t}{\Delta s^2} = \frac{1}{2} \qquad \Leftrightarrow \qquad \Delta s = \pm\sqrt{2k\Delta t} \tag{6}$$

and the following expression is then obtained:

$$A_j^{n+\Delta t} = \frac{1}{2}A_{j+\Delta s}^n + \frac{1}{2}A_{j-\Delta s}^n. \tag{7}$$

Other values can be imposed as long as they are less than the limit for stability that is $\frac{1}{2}$. Examples used in this paper are $\frac{1}{4}$ and $\frac{1}{6}$, where the latter is the value that leads to the highest accuracy in the explicit scheme [7]. If the imposed stability number is $\frac{1}{6}$ the solver

$$A_j^{n+\Delta t} = \frac{1}{6}A_{j+\Delta s}^n + \frac{2}{3}A_j^n + \frac{1}{6}A_{j-\Delta s}^n \tag{8}$$

is then obtained, where Δs is determined as

$$k\frac{\Delta t}{\Delta s^2} = \frac{1}{6} \qquad \Leftrightarrow \qquad \Delta s = \pm\sqrt{6k\Delta t}. \tag{9}$$

The new scheme is stable by design, since it imposes a fixed value for the stability coefficient below the stability limit. This information is then used to determine a new grid, and the values at the new grid are obtained by interpolation from the original grid. In practice, when the stability coefficient reaches values that lead to an unstable explicit scheme, stability in the new scheme is achieved by extending the stencil ($\Delta s > \Delta x$).

Although this work is mainly concerned with the case of a constant diffusion coefficient, some results with a variable coefficient will be presented in Section 5 to illustrate the potential advantages of the new scheme in dealing with non-linear problems. For the more general case of a diffusion coefficient that changes in space, the new scheme can be written as

$$\begin{aligned} A_j^{n+\Delta t} = A_j^n &+ \frac{\Delta t}{2}k_{j+\Delta s_+/2}\left(\frac{1}{\Delta s_+^2} + \frac{1}{\Delta s_+\Delta s_-}\right)\left(A_{j+\Delta s_+}^n - A_j^n\right) \\ &- \frac{\Delta t}{2}k_{j-\Delta s_-/2}\left(\frac{1}{\Delta s_+\Delta s_-} + \frac{1}{\Delta s_-^2}\right)\left(A_j^n - A_{j-\Delta s_-}^n\right), \end{aligned} \tag{10}$$

where Δ_{s_+} and Δ_{s_-} are, respectively, the distance that corresponds to larger and smaller values of the space discretization index.

To obtain Eq. (10), a spatial partial derivative at point j of a variable D is estimated as

$$\left(\frac{\partial D}{\partial x}\right)_j \simeq \frac{1}{2}\left(\frac{D_{j+\Delta s_+} - D_j}{\Delta s_+} + \frac{D_j - D_{j-\Delta s_-}}{\Delta s_-}\right). \tag{11}$$

It is easy to see that for the constant diffusion case $\Delta s_+ = \Delta s_-$ and Eq. (10) reduces to Eq. (4).

By imposing a constant value to the stability number β, Δs_+ and Δs_- can be determined from the expressions

$$\Delta s_-^2 = \frac{1}{2}(k_- + k_+)\frac{k_-}{k_+}\frac{\Delta t}{\beta} \tag{12}$$

$$\Delta s_+^2 = \frac{1}{2}(k_- + k_+)\frac{k_+}{k_-}\frac{\Delta t}{\beta}. \tag{13}$$

These two relations and Eq. (10) can be used iteratively to find the optimal Δs_+ and Δs_-. In this case k_+ and k_- can, for example, be equal to k_j at the first iteration and for the following iterations we have:

$$k_- = k_{j-\Delta s_-/2} \qquad \bigwedge \qquad k_+ = k_{j+\Delta s_+/2}. \tag{14}$$

For a diffusion coefficient that changes in time as well as in space, Eq. (10) can also be used with the diffusion coefficient being taken at time step n. It is not complicated to extend this type of scheme to diffusion equations with more than one dimension using methods based on alternating directions. To include source and sink terms on the rhs of the diffusion equation is also not problematic. It can be seen that this method is very general and can probably be applied successfully to solve, in a stable manner, other partial differential equations.

3. A DERIVATION OF THE DIFFUSION EQUATION

Here a simple derivation of the diffusion equation based on the random walk approach is presented. Let N_j^n be the number of particles at point j and time step n, and assume that the probability of particles moving to the left or to the right is the same, equal to p and smaller than $\frac{1}{2}$. Then at time step $n + \Delta t$,

$$N_j^{n+\Delta t} = pN_{j+\Delta s}^n + (1 - 2p)N_j^n + pN_{j-\Delta s}^n. \tag{15}$$

This relation can also be written in terms of a generic property A:

$$A_j^{n+\Delta t} = pA_{j+\Delta s}^n + (1 - 2p)A_j^n + pA_{j-\Delta s}^n. \tag{16}$$

Expanding in Taylor series, after some simple algebra and neglecting the higher order terms, the following expression is obtained:

$$\frac{\partial A}{\partial t} = \frac{p\Delta s^2}{\Delta t}\frac{\partial^2 A}{\partial x^2}. \tag{17}$$

Assuming that when Δt, $\Delta s \to 0$, $\lim(p\Delta s^2)/(\Delta t) = k$ and k is a constant, Eq. (17) represents the diffusion equation, with a constant diffusion coefficient.

More formal derivations of the diffusion equation based on the random walk approach can be found in, among others [4, 8]. In any case, these more formal derivations are ultimately also based on the assumption that when Δt, $\Delta s \to 0$, $\lim(p\Delta s^2)/(\Delta t) = k$. A discrete version of this assumption plays an important role in the development of the scheme presented in this paper because with this method it is assumed that $p\Delta s^2/\Delta t = k$ is true for any Δt and Δs and not only when Δt, $\Delta s \to 0$.

4. DISCUSSION

There is also an analogy between the new diffusion scheme and the semi-Lagrangian method used to solve the advection equation. Semi-Lagrangian methods have been widely used in atmospheric models in recent years; detailed reviews can be found in [10] and [12]. The idea of solving the diffusion equation based on concepts related to advection schemes is not new. In [9] and [11] it is shown how a positive definite advection transport algorithm can be successfully used to solve the diffusion and the advection–diffusion equation. Much of their underlying theory could possibly be adapted to devise a diffusion scheme similar in its stability properties to the one presented in this paper.

An important point is that using the new scheme when $\Delta s < \Delta x$ it should be possible to obtain the explicit solver algorithm of Eq. (2). In fact, if $\Delta s < \Delta x$ and the new scheme is used with a quadratic interpolation and with $\beta = \frac{1}{2}$ the expression

$$\begin{aligned} A_j^{n+\Delta t} &= \frac{1}{2}\left(\frac{\delta(\delta-1)}{2}A_{j+\Delta x}^n + (1-\delta^2)A_j^n + \frac{\delta(\delta+1)}{2}A_{j-\Delta x}^n\right) \\ &\quad + \frac{1}{2}\left(\frac{\delta(\delta-1)}{2}A_{j-\Delta x}^n + (1-\delta^2)A_j^n + \frac{\delta(\delta+1)}{2}A_{j+\Delta x}^n\right) \end{aligned} \tag{18}$$

is obtained, where $\delta = |\Delta s|/\Delta x$. After some simple algebra,

$$A_j^{n+\Delta t} = \frac{1}{2}\delta^2 A_{j+\Delta x}^n + (1-\delta^2)A_j^n + \frac{1}{2}\delta^2 A_{j-\Delta x}^n, \tag{19}$$

which is, taking into account the definition of δ, the same as the explicit diffusion solver shown in Eq. (2).

In principle the new scheme presented in this work is stable by design, since it imposes a fixed value for a stability coefficient β, below the stability limit, and uses this information in order to determine a new grid. The values of the variables at the new grid are then obtained by interpolation from the original grid. However, a more detailed study is presented here in order to analyse the stability of the new scheme and the behaviour of the amplification factor compared with other schemes.

In order to simplify this study only a particular configuration of the scheme is analysed: the one that corresponds to a linear interpolation and to Δs between Δx and $2\Delta x$, i.e.,

$$\Delta s = \Delta x + \varepsilon \qquad \text{with } 0 < \varepsilon < \Delta x. \tag{20}$$

With linear interpolation,

$$A_{j+\Delta s} = (1-\eta)A_{j+\Delta x} + \eta A_{j+2\Delta x} \tag{21}$$

$$A_{j-\Delta s} = (1-\eta)A_{j-\Delta x} + \eta A_{j-2\Delta x} \tag{22}$$

with

$$\eta = \frac{\varepsilon}{\Delta x}. \tag{23}$$

In this case the algorithm for the new scheme can be written as

$$A_j^{n+\Delta t} = A_j^n + k\frac{\Delta t}{\Delta s^2}\left(A_{j+\Delta x}^n - 2A_j^n + A_{j-\Delta x}^n\right) + k\frac{\Delta t}{\Delta s^2}\eta\left(A_{j+2\Delta x}^n - A_{j+\Delta x}^n - A_{j-\Delta x}^n + A_{j-2\Delta x}^n\right) \tag{24}$$

or after some simple algebra

$$A_j^{n+\Delta t} = A_j^n + k\frac{\Delta t}{\Delta x^2}\left(A_{j+\Delta x}^n - 2A_j^n + A_{j-\Delta x}^n\right) + k\frac{\Delta t}{\Delta x^2}\left(\frac{1}{(1+\eta)^2} - 1\right)\left(A_{j+\Delta x}^n - 2A_j^n + A_{j-\Delta x}^n\right) + k\frac{\Delta t}{\Delta x^2}\frac{\eta}{(1+\eta)^2}\left(A_{j+2\Delta x}^n - A_{j+\Delta x}^n - A_{j-\Delta x}^n + A_{j-2\Delta x}^n\right). \tag{25}$$

Expanding the variable discrete values in Taylor series and neglecting the higher order terms the equation

$$\frac{\partial A}{\partial t} = k\frac{\partial^2 A}{\partial x^2} + \left(\frac{3\eta+1}{(1+\eta)^2} - 1\right)k\frac{\partial^2 A}{\partial x^2} \tag{26}$$

is obtained, or

$$\frac{\partial A}{\partial t} = \gamma k\frac{\partial^2 A}{\partial x^2} \tag{27}$$

with

$$\gamma = \frac{3\eta+1}{(1+\eta)^2}. \tag{28}$$

It is quite straightforward to see that for $\eta = 0$ (which corresponds to $\Delta s = \Delta x$) and for $\eta = 1$ ($\Delta s = 2\Delta x$), $\gamma = 1$ and the equation reduces to the normal diffusion equation. Since η is between 0 and 1, γ is never larger than 1.125 and, for example, for $\eta = 0.5$, $\gamma = 1.11111$.

To analyse the stability of this particular scheme the amplification factor for a Fourier mode in space is determined. The amplification factor, for the new scheme in this particular configuration, is

$$\psi = 1 - 4k\frac{\Delta t}{\Delta s^2}\sin^2\left(K\frac{\Delta x}{2}\right) + 2k\frac{\Delta t}{\Delta s^2}\eta\left[\left(8\cos^2\left(K\frac{\Delta x}{2}\right) - 10\right)\cos^2\left(K\frac{\Delta x}{2}\right) + 2\right], \tag{29}$$

where K is the wave number.

If $\eta = 0$, Eq. (29) becomes the amplification factor of the common explicit solver. The following simplified extreme cases can be analysed. For $\cos^2(K\Delta x/2) = 1$, $\psi = 1$ and for $\sin^2(K\Delta x/2) = 1$ the stability condition leads to

$$\beta(1-\eta) \le \frac{1}{2}, \tag{30}$$

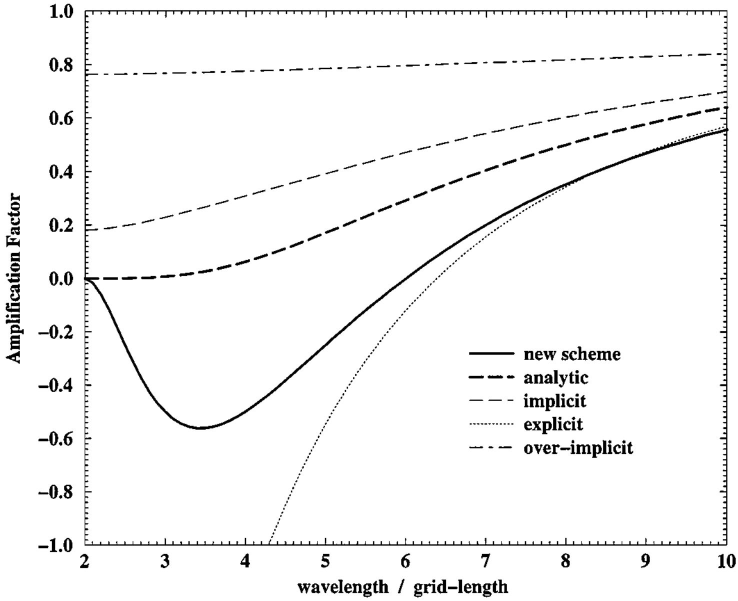

FIG. 1. The amplification factor versus the wavelength divided by the grid length, for the new, the explicit, and the implicit schemes. Results obtained with $\beta = \frac{1}{2}$, which corresponds (assuming $\Delta s - \Delta x = 0.5\Delta x$) to $\alpha = 1.12$. Also shown are the analytic solution and an over-implicit scheme with an implicitness factor of 4.

which is always true since by design of the scheme

$$\beta \leq \frac{1}{2} \quad \bigwedge \quad 0 \leq \eta \leq 1. \tag{31}$$

To investigate in greater detail the properties of this scheme, the amplification factor of this and other well-known schemes is plotted as a function of the wavelength divided by the grid length, for different values of β. It is always assumed that $\Delta s - \Delta x = 0.5\Delta x$.

In Fig. 1 the amplification factor is shown for the new, the explicit and the implicit schemes. These results were obtained for $\beta = \frac{1}{2}$, which corresponds to a value of the normal stability coefficient $\alpha = 1.12$ (assuming $\Delta s - \Delta x = 0.5\Delta x$). Also shown are the results for the analytic solution and an over-implicit scheme. The implicit scheme takes the values of the variables on the rhs of Eq. (1) at time-step $n + \Delta t$, which corresponds to an implicitness factor of 1, and the over-implicit scheme uses an implicitness factor of 4 [1]. It can be seen that, since the stability coefficient α is above 0.5, the explicit solver gives an unstable solution for wavelengths smaller than about $4.3\Delta x$. For this case the implicit scheme provides the best results when compared with the analytical solution. However, the new scheme is reasonably well behaved for wavelengths larger than about $6\Delta x$. The results for the over-implicit scheme are represented in these figures to show that, although stable, this type of scheme can be highly inaccurate.

In Fig. 2 the same is shown, but in this case for a value of $\beta = \frac{1}{4}$, which corresponds to $\alpha = 0.5625$. Again, the explicit scheme is above its stability limit and gives an amplification factor less than -1 for wavelengths smaller than about $2.55\Delta x$. In this case the new scheme, when compared with the analytic solution, is clearly superior to the implicit scheme (except for wavelengths close to $2\Delta x$).

In Fig. 3 the same is shown but for $\beta = \frac{1}{6}$ and $\alpha = 0.375$. In this case the explicit scheme is always stable. The new scheme is again better than the implicit and the explicit schemes

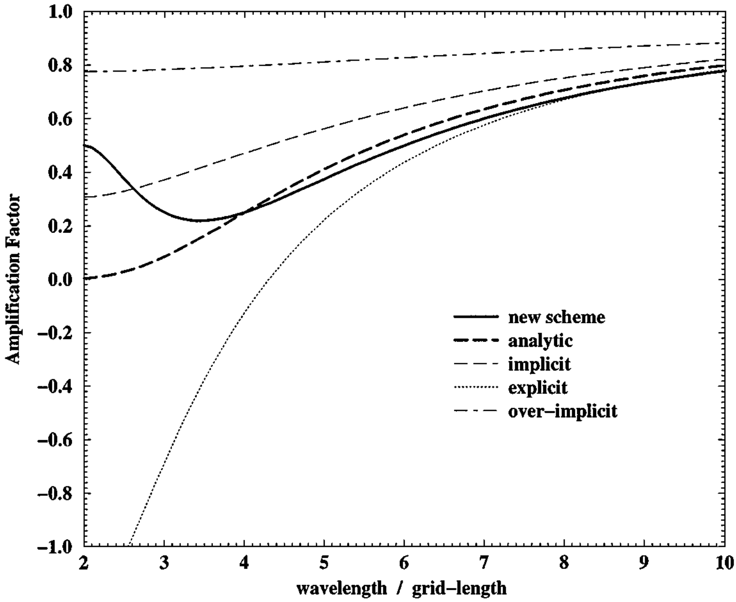

FIG. 2. Same as Fig. 1 but for $\beta = \frac{1}{4}$ and $\alpha = 0.5625$.

for most of the wavelengths shown in the figure. The results of the new scheme are actually very similar to the analytic solution for wavelengths above $5.5\Delta x$.

Figure 4 shows the amplification factor versus the wavelength divided by the grid length, for the analytic solution, the new scheme, the implicit scheme, the Crank–Nicholson scheme, and the Dufort–Frankel scheme. The Crank–Nicholson scheme is obtained when the spatial diffusion term is averaged in time between time steps n and $n + \Delta t$, which

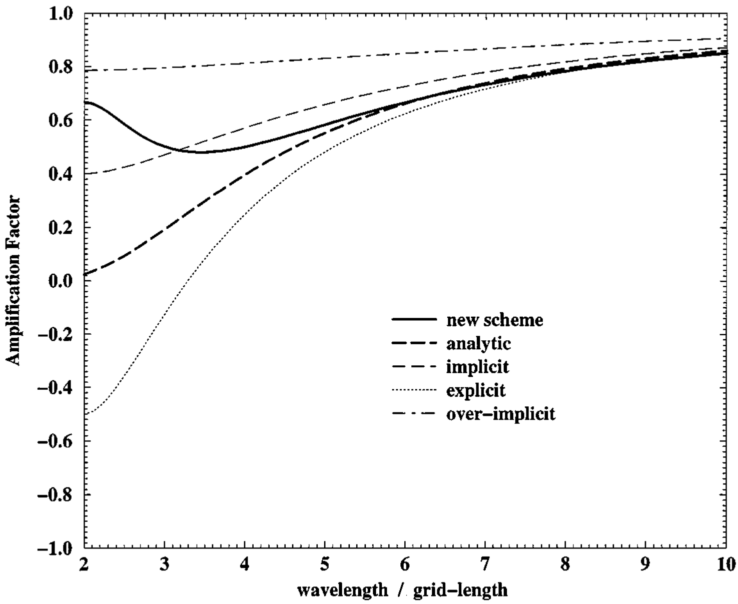

FIG. 3. Same as Fig. 1 but for $\beta = \frac{1}{6}$ and $\alpha = 0.375$.

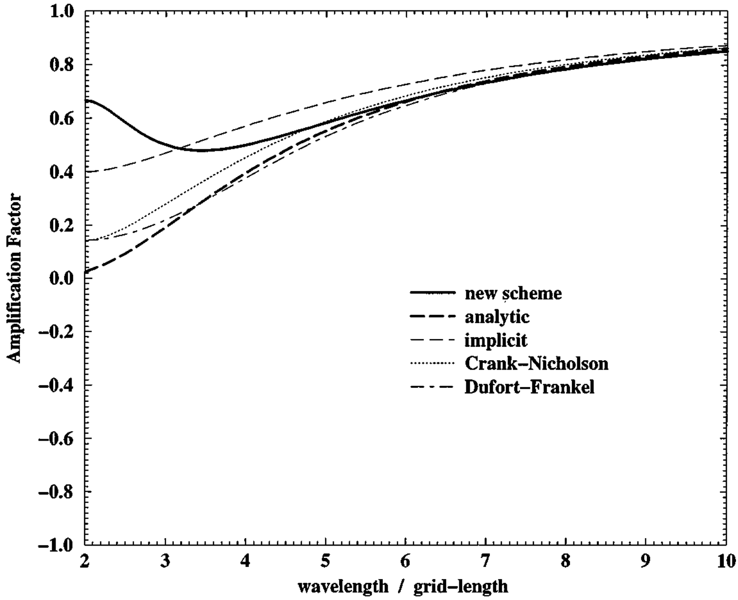

FIG. 4. The amplification factor versus the wavelength divided by the grid length, for the analytic solution, the new scheme, the implicit scheme, the Crank–Nicholson scheme, and the Dufort–Frankel scheme. Results were obtained with $\beta = \frac{1}{6}$ and $\alpha = 0.375$.

corresponds to an implicitness factor of 0.5. The Dufort–Frankel scheme is a three-time-level scheme slightly altered in order to have, on the rhs of the discretized equation, the value of the variable at the central point as an average between time steps $n - \Delta t$ and $n + \Delta t$. These results are obtained with $\beta = \frac{1}{6}$ and $\alpha = 0.375$. The Dufort–Frankel scheme provides the best results when compared with the analytic solution. However, above wavelength $5\Delta x$ the new scheme gives results that are better than the ones obtained with the Crank–Nicholson scheme and comparable with the ones obtained with the Dufort–Frankel scheme.

In Fig. 5 the same as in Fig. 4 is shown, but for $\beta = \frac{1}{4}$ and $\alpha = 0.5625$. The results obtained with the Crank–Nicholson scheme are quite superior to those of any other scheme and compare very well with the analytic solution. The new scheme, however, gives results that are quite reasonable above wavelength $4\Delta x$ and are much better than the ones obtained with the Dufort–Frankel scheme. In this case the results of the Dufort-Frankel scheme have some odd features, which are well known [6].

In summary it can be said that in general the new scheme is reasonably accurate when compared with analytic solutions and other numerical schemes. However, for wavelengths close to $2\Delta x$, the new scheme does not seem to provide very satisfactory results.

The issue of conservation is one to which special attention should be paid. The new scheme for the case of a constant diffusion coefficient does not have conservation problems: it is straightforward to show that the new scheme with linear interpolation is conservative for a constant diffusion coefficient as long as the values of the variables close to the boundaries are set in an appropriate manner. For the case of a variable diffusion coefficient the problem is more complicated, but since this paper is mainly about the constant diffusion coefficient case, this will not be explored any further. Also, in the applications that are being considered here, the numerical stability problem is more important than the issue of conservation.

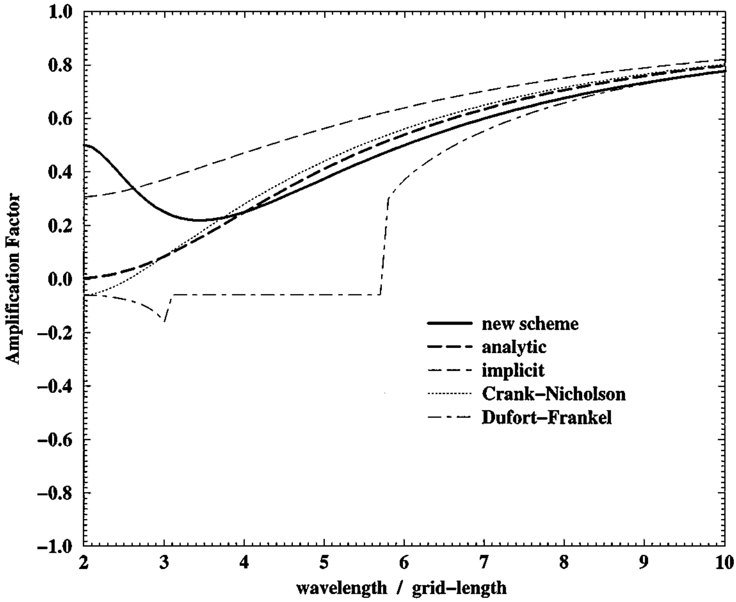

FIG. 5. Same as Fig. 4 but for $\beta = \frac{1}{4}$ and $\alpha = 0.5625$.

A potential problem with the new scheme is how to impose boundary conditions. The new scheme will have a problem every time the distance Δs is larger than the distance to the boundary. A simple solution is this: every time the distance Δs (and the chosen interpolation scheme) implies that the value of the variable at points outside the boundaries has to be defined, the value of the variable at these points is set to be equal to the boundary value. This assumption has been tested and has proved to be quite realistic for the surface boundary condition of the vertical turbulent diffusion equation in atmospheric models.

5. SOME SIMPLE TESTS

5.1. *A Comparison with an Analytical Solution*

For the simplified case of a constant diffusion coefficient and a delta function at initial time $t = 0$ s, the diffusion equation has an analytical solution. The analytical solution at time $t = 100$ s is used as the initial condition of the numerical integrations, and the solutions of these simulations after 100 and 500 s are then compared against the analytical solutions at the corresponding times.

Figure 6 shows the initial state, the analytical solution at time $t = 200$ s, and two numerical solutions obtained with the new method 100 s after the initial state: one using linear interpolation and the other using cubic interpolation, both with $\beta = \frac{1}{2}$. In this case the diffusion coefficient is $10\,\mathrm{m}^2\,\mathrm{s}^{-1}$. The numerical integrations use a grid space of 1 m and a time step of 1 s. As can be seen, both numerical integrations, with the linear or cubic interpolation, have reasonable results when compared with the analytical solution. However, the simulation that uses cubic interpolation is clearly more accurate than the one with linear interpolation and is almost indistinguishable from the analytical solution.

In order to perform a more systematic study several runs for the same situation were performed with the new scheme, with linear and cubic interpolations, and with the implicit scheme.

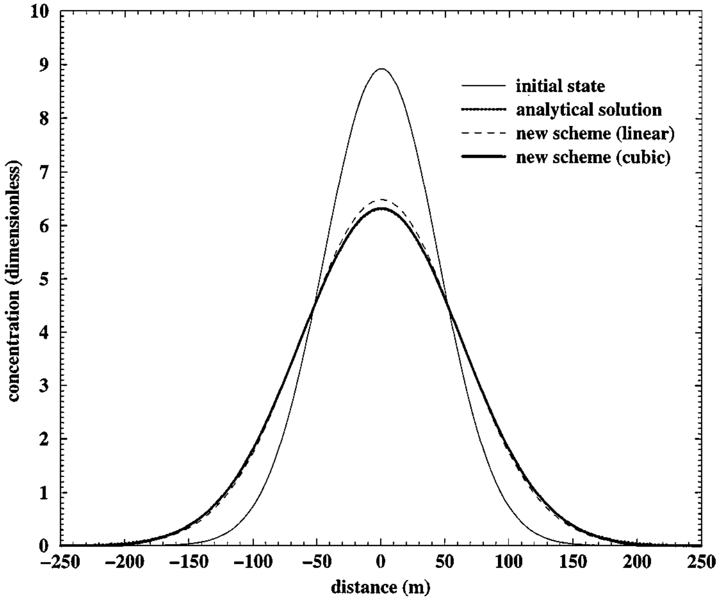

FIG. 6. The initial state, the analytical solution at time $t = 200$ s, and two numerical solutions obtained with the new method 100 s after the initial state, one using linear interpolation and the other using cubic interpolation.

In Table 1 the results for the new scheme with linear interpolation are shown. The results correspond to different values of $\beta\,(\frac{1}{2}, \frac{1}{4}$, and $\frac{1}{6})$, different values of the diffusion coefficient (1 and $10\,\mathrm{m}^2\,\mathrm{s}^{-1}$), and different run times (100 and 500 s). For each of these different experiments, the root mean square (RMS) error, when compared with the analytical solution, was computed. In Table 2 the same is shown but for the new scheme with cubic interpolation.

It can be seen that the scheme with cubic interpolation is in general more accurate than that with linear interpolation. Another aspect, which is particularly obvious with the cubic

TABLE 1

Results with the New Scheme with Linear Interpolation, for the Case of a Constant Diffusion Coefficient (see text for details)

β	k ($\mathrm{m}^2\,\mathrm{s}^{-1}$)	Time (s)	RMS error
$\frac{1}{2}$	1	100	9.65522E-2
$\frac{1}{2}$	1	500	1.18139E-1
$\frac{1}{4}$	1	100	1.00434E-3
$\frac{1}{4}$	1	500	4.23027E-4
$\frac{1}{6}$	1	100	3.26799E-2
$\frac{1}{6}$	1	500	4.13800E-2
$\frac{1}{2}$	10	100	6.64590E-3
$\frac{1}{2}$	10	500	7.56742E-3
$\frac{1}{4}$	10	100	2.97326E-3
$\frac{1}{4}$	10	500	3.35876E-3
$\frac{1}{6}$	10	100	1.42019E-3
$\frac{1}{6}$	10	500	1.80493E-3

TABLE 2
Results with the New Scheme with Cubic Interpolation, for the Case of a Constant Diffusion Coefficient (see text for details)

β	k ($m^2\ s^{-1}$)	Time (s)	RMS error
$\frac{1}{2}$	1	100	2.14781E-3
$\frac{1}{2}$	1	500	9.06875E-4
$\frac{1}{4}$	1	100	1.00434E-3
$\frac{1}{4}$	1	500	4.23027E-4
$\frac{1}{6}$	1	100	3.98937E-5
$\frac{1}{6}$	1	500	3.21637E-5
$\frac{1}{2}$	10	100	1.13189E-3
$\frac{1}{2}$	10	500	4.77263E-4
$\frac{1}{4}$	10	100	5.63754E-4
$\frac{1}{4}$	10	500	2.34189E-4
$\frac{1}{6}$	10	100	5.66400E-6
$\frac{1}{6}$	10	500	1.56124E-5

interpolation, is that the more accurate results are obtained when $\beta = \frac{1}{6}$. This is in agreement with the fact that with the explicit scheme the most accurate results are obtained when the stability coefficient is $\frac{1}{6}$ [7].

Comparing the previous tables with Table 3, where similar results are shown for the implicit scheme, it can be seen that the implicit scheme is always less accurate than the new scheme with cubic interpolation. In particular, the new scheme with cubic interpolation and $\beta = \frac{1}{6}$ is often 1 or 2 orders of magnitude more accurate than the implicit scheme.

Although all the results shown are from runs that were performed with a domain size of 10,000 points, the same simulations were also performed with domains of 1,000 and 100,000 points. However, the results of these runs are not shown because no major sensitivity to the domain size was detected.

The conservation issue was also examined in this study. These results are not shown because, although no special care was taken with the values close to the boundaries, the difference between the total initial concentration and the final one was usually less than 0.001% for all the runs with the new scheme.

TABLE 3
Results with the Implicit Scheme for the Case of a Constant Diffusion Coefficient (see text for details)

k ($m^2\ s^{-1}$)	Time (s)	RMS error
1	100	3.50450E-3
1	500	1.52026E-3
10	100	1.69009E-3
10	500	7.01931E-4

5.2. *A System of Two Non-linear Diffusion Equations*

To illustrate the potential advantages of the new scheme, the system of equations

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial z} k \frac{\partial u}{\partial z}$$
$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} k \frac{\partial \theta}{\partial z} \tag{32}$$

is considered [2], where u is the wind speed and θ is the potential temperature. The diffusion coefficient is

$$k = l^2 \left| \frac{\partial u}{\partial z} \right| (1 + b|\mathrm{Ri}|)^n, \tag{33}$$

where l is a mixing length and Ri is the Richardson number defined by

$$\mathrm{Ri} = \frac{g(\partial\theta/\partial z)}{\theta_0(\partial u/\partial z)^2}, \tag{34}$$

where g is the acceleration of gravity and θ_0 is a constant. The values that are used for the constants b and n are [2] $n = -2$ and $b = 5$ for $\mathrm{Ri} > 0$ and $n = 1/2$ and $b = 20$ for $\mathrm{Ri} < 0$. This type of equation is often encountered in problems related to the parametrization of turbulence in models of geophysical flows. This particular set of equations has been used to parametrize vertical turbulent mixing in global atmospheric models [2].

A simplified situation is considered: a one-dimensional domain with 10^5 points separated by a grid space of 1 m. The initial values for u and θ are $10\,\mathrm{m\,s^{-1}}$ and 310 K, respectively, in every point of the domain except in the middle point, where u is $0\,\mathrm{m\,s^{-1}}$ and θ is 250 K.

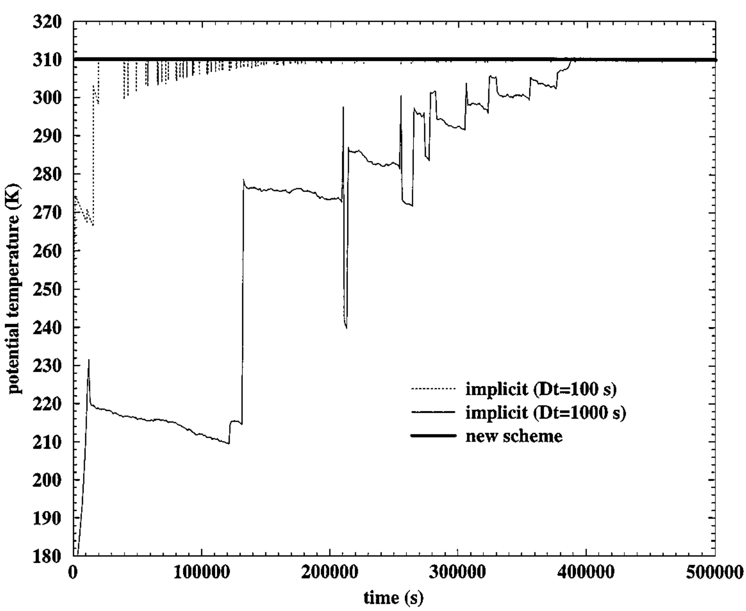

FIG. 7. Time evolution of θ in the middle point of the domain for the first 500,000 s, obtained with the implicit method (time steps of 100 and 1,000 s) and with the new scheme.

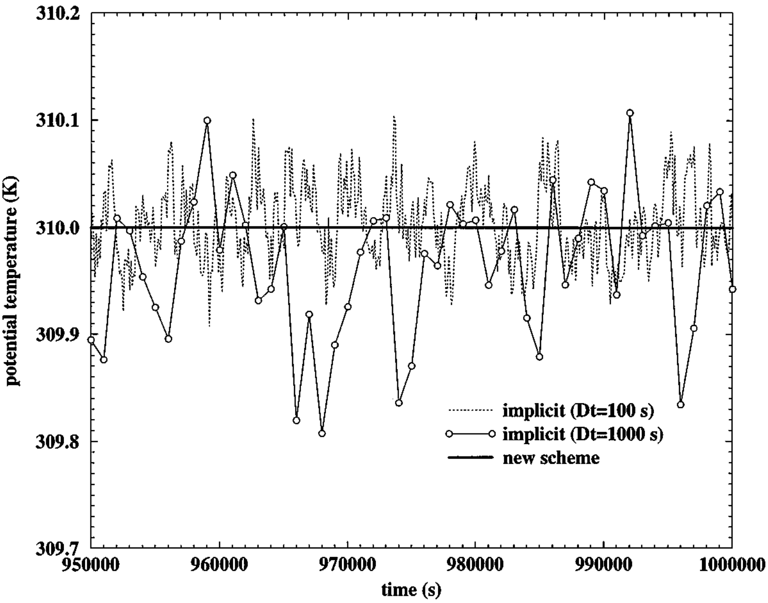

FIG. 8. Same as Fig. 7, but for the last 50,000 s of a run of 1,000,000 s.

The system is solved by two different methods: (i) a method that will be referred to as “implicit” where on the rhs the mean variables are taken implicitly and the diffusion coefficient explicitly in time, and (ii) the method presented in this paper, with $\beta = \frac{1}{2}$ and a linear interpolation scheme. Since in this situation the diffusion coefficient varies in space and time, Eqs. (10), (12), and (13) will be used, as shown in Section 2, with three iterations.

As can be seen in Fig. 7, where the time evolution of θ in the middle point of the domain is shown for the first 500,000 s, the solution obtained with the implicit method is noisy for time steps of 100 and 1,000 s. The amplitude of the initial oscillation increases with the time step. The results with the new scheme are better. A constant solution is obtained, as is more clear from Fig. 8.

In Fig. 8 the potential temperature evolution from 950,000 to 1,000,000 s is shown. It can be seen that the solutions obtained with the implicit method are always noisy. Again the amplitude of the oscillations increases with the time step. With the new scheme a solution with a constant value of 310 K is obtained.

With the new method the simulations were performed with a time step of 1,000 s, but the results for the new scheme are independent of the time step used (at least in the range 1–10,000 s). This test shows that the new method has fewer numerical stability problems than the implicit method.

6. CONCLUSIONS

In this paper a new method to solve the one-dimensional diffusion equation has been presented. This new scheme is stable by design, since it imposes a fixed value for a stability coefficient below the stability limit and uses this information to determine a new grid. The values of the variables at the new grid are then obtained by interpolation from the original grid. The new method is quite general and can be used to solve other partial differential equations.

An analysis of the amplification factor of some particular configurations of this scheme shows that the new method is not only stable but often more accurate than other, commonly used, numerical methods. It is also shown that the explicit scheme can be obtained as a particular configuration of the new method presented in this paper.

The results of the new scheme compare well with analytical solutions, for the simplified case of a constant diffusion coefficient. Some configurations of the new scheme can actually provide results that are always more accurate than with the implicit method.

A study with a system of two non-linear diffusion equations for wind and potential temperature shows that the new method is more stable than a more traditional implicit scheme, where on the rhs the mean variables are taken implicitly and the diffusion coefficient is taken explicitly in time.

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