

## Abstract

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. The method, that 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.

## 1. INTRODUCTION

In atmospheric models the 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 (*Beljaars, 1991, Girard and Delage, 1990*). This type of problem is one of the reasons why the time step of climate models cannot be significantly increased (*Williamson, 1996*). Non-linear diffusion equations are used to model a variety of different phenomena, from engineering flows (*Oran and Boris, 1987*) and magnetohydrodynamics (*Potter, 1973*) to insect dispersal (*Murray, 1993*). These models suffer from similar types of numerical stability problems and a method that would “solve” 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 this case a fully implicit method cannot be used. In practice, the problem is often solved with an implicit formulation for  $A$  and an explicit formulation for  $k$ , but such a scheme is not necessarily stable in all circumstances (*Beljaars, 1991*). Due to the stability problems a scheme usually referred to as “more-than-implicit” or “over-implicit”, which corresponds to an implicitness factor larger than 1 (*Beljaars, 1991*), has been used in atmospheric models (*Girard and Delage, 1990; Jarraud et al., 1985*).

The aim of this paper is to present a new type of algorithms 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 section 5.1 the results of simple tests are shown. Although this work is mainly concerned with the constant diffusion coefficient case, in section 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:

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

Discretizing the one-dimensional diffusion equation in space and explicitly in time (assuming that the diffusion coefficient  $k$  is constant) gives:

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

where  $\Delta t$  is the time step,  $\Delta x$  is the grid length,  $n$  is the time discretization index and  $j$  the space discretization index. The stability coefficient is:

$$\alpha = k \frac{\Delta t}{\Delta x^2} \quad (3)$$

A simple stability analysis shows that if  $\alpha \leq 1/2$  eq. (2) is stable and if  $\alpha > 1/2$  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:

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

To obtain eq. (4) the spatial partial derivative is approximated by a finite difference along the distance  $\Delta s$ , that does not have to be equal to the grid length and can be determined by imposing a fixed stability number  $\beta \leq 1/2$ :

$$k \frac{\Delta t}{\Delta s^2} = \beta \quad \Leftrightarrow \quad \Delta s = \pm \sqrt{\frac{k \Delta t}{\beta}} \quad (5)$$

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  $1/2$  it is:

$$k \frac{\Delta t}{\Delta s^2} = \frac{1}{2} \quad \Leftrightarrow \quad \Delta s = \pm \sqrt{2k \Delta t} \quad (6)$$

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 1/2. Examples used in this paper are 1/4 or 1/6 that is the value that leads to the highest accuracy in the explicit scheme (Richtmyer and Morton, 1967). If the imposed stability number is 1/6 the following solver is then obtained:

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

where  $\Delta s$  is determined as:

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

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 in order 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:

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

where  $\Delta s_+$  and  $\Delta s_-$  are, respectively, the distance that corresponds to larger and smaller values of the space discretization index.

To obtain equation (10) a spatial partial derivative at point  $j$  of a variable  $D$  is estimated as:

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

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

By imposing a constant value to the stability number  $\beta$ ,  $\Delta s_+$  and  $\Delta s_-$  can be determined from the following expressions:

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

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

These two relations and equation (10) can be used iteratively in order to find the optimal  $\Delta s_+$  and  $\Delta s_-$ . In this case  $k_+$  and  $k_-$  can, for example, be equal to  $k_j$  at the first iteration and for the following iterations it is:

$$k_- = k_{j-\Delta s_- / 2} \quad \wedge \quad k_+ = k_{j+\Delta s_+ / 2} \quad (14)$$

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 schemes 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  $1/2$ . Then at time step  $n+1$ :

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

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

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

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

$$\frac{\partial A}{\partial t} = \frac{p \Delta s^2}{\Delta t} \frac{\partial^2 A}{\partial x^2} \quad (17)$$

Assuming that when  $\Delta t, \Delta s \rightarrow 0$ ,  $\lim(p\Delta s^2)/(\Delta t) = k$  and  $k$  is a constant, then 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, *Murray* (1993) or *Sorbjan* (1989). In any case, these more formal derivations are ultimately also based on the assumption that when  $\Delta t, \Delta s \rightarrow 0$ , then  $\lim(p\Delta s^2)/(\Delta t) = k$ . A discrete version of this assumption plays an important role in the development of the scheme that is presented in this paper because with this method it is assumed that  $p\Delta s^2/\Delta t = k$  is true for any  $\Delta t$  and  $\Delta s$  and not only when  $\Delta t, \Delta s \rightarrow 0$ .

#### 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 and detailed reviews can be found in *Smolarkiewicz and Pudykiewicz* (1992) and *Staniforth and Cote* (1991). The idea of solving the diffusion equation based on concepts related to advection schemes is not new. In *Smolarkiewicz and Clark* (1986) and *Smolarkiewicz and Margolin* (1998) 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  $\beta = 1/2$  the following expression is obtained:

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

where  $\delta = |\Delta s|/\Delta x$ . After some simple algebra:

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

which is, taking into account the definition of  $\delta$ , 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  $\beta$ , 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 a  $\Delta s$  between  $\Delta x$  and  $2\Delta x$ , i.e.:

$$\Delta s = \Delta x + \varepsilon \quad \text{with} \quad 0 < \varepsilon < \Delta x \quad (20)$$

With linear interpolation:

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

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

with

$$\eta = \frac{\varepsilon}{\Delta x} \quad (23)$$

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

$$\begin{aligned} A_j^{n+\Delta t} = & A_j^n + k \frac{\Delta t}{\Delta s^2} (A_{j+\Delta x}^n - 2A_j^n + A_{j-\Delta x}^n) \\ & + k \frac{\Delta t}{\Delta s^2} \eta (A_{j+2\Delta x}^n - A_{j+\Delta x}^n - A_{j-\Delta x}^n + A_{j-2\Delta x}^n) \end{aligned} \quad (24)$$

or after some simple algebra

$$\begin{aligned} A_j^{n+\Delta t} = & A_j^n + k \frac{\Delta t}{\Delta x^2} (A_{j+\Delta x}^n - 2A_j^n + A_{j-\Delta x}^n) \\ & + k \frac{\Delta t}{\Delta x^2} \left( \frac{1}{(1+\eta)^2} - 1 \right) (A_{j+\Delta x}^n - 2A_j^n + A_{j-\Delta x}^n) \\ & + k \frac{\Delta t}{\Delta x^2} \frac{\eta}{(1+\eta)^2} (A_{j+2\Delta x}^n - A_{j+\Delta x}^n - A_{j-\Delta x}^n + A_{j-2\Delta x}^n) \end{aligned} \quad (25)$$

Expanding the variable discrete values in Taylor series and neglecting the higher order terms the following equation is obtained:



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

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  $\eta$  is between 0 and 1,  $\gamma$  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:

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

where  $K$  is the wave number.

If  $\eta = 0$  eq.(29) becomes the amplification factor of the common explicit solver. First of all, 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 condition that the amplification factor must be less than 1 leads to:

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

which is always true since by design of the scheme

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

To investigate in more detail the properties of the 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  $\beta$ . 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  $\beta=1/2$  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 with an implicitness factor of 4 (Beljaars 1991). It can be seen that, since the stability coefficient  $\alpha$  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" are represented in these figures to show that, although stable, this type of schemes can be highly inaccurate.

In fig.2 the same is shown, but in this case for a value of  $\beta=1/4$ , that 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  $\beta=1/6$  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 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 and also for the Crank-Nicholson and the Dufort-Frankel schemes. These results are obtained with  $\beta=1/6$  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  $\beta=1/4$  and  $\alpha=0.5625$ . The results obtained with the Crank-Nicholson scheme are quite superior to 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 (Potter, 1973).

As a 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.

A potential problem with the new scheme is how to impose boundary conditions. The new scheme will have a problem every time the distance  $\Delta s$  is larger than the distance to the boundary. A simple solution is: every time the distance  $\Delta s$  (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 s and 500 s are then compared against the analytical solutions at the corresponding times.

Fig. 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 cubic interpolation, both with  $\beta=1/2$ . In this case the diffusion coefficient is  $10 \text{ m}^2 \text{ s}^{-1}$ . 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 the cubic interpolation is clearly more accurate than the one with the 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.

In table I the results for the new scheme with linear interpolation are shown. The results correspond to different values of  $\beta$  (1/2, 1/4 and 1/6), different values of the diffusion coefficient (1 and  $10 \text{ m}^2 \text{ s}^{-1}$ ) and different run-times (100 s and 500 s). For each one of these different experiments, the Root Mean Square (RMS) error, when compared with the analytical solution, was computed. In table II the same is shown but for the new scheme with cubic interpolation.

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

results are obtained when  $\beta=1/6$ . This is in agreement with the fact that with the explicit scheme the most accurate results are obtained when the stability coefficient is  $1/6$  (*Richtmyer and Morton, 1967*).

Comparing the previous tables with table III 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  $\beta=1/6$  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 10000 points, the same simulations were also performed with domains of 1000 and 100000 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. The 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.

## 5.2. A System of Two Non-Linear Diffusion Equations

To illustrate the potential advantages of the new scheme, the following system of equations is considered (*Girard and Delage, 1990*):

$$\begin{cases} \frac{\partial u}{\partial t} = \frac{\partial}{\partial z} k \frac{\partial u}{\partial z} \\ \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} k \frac{\partial \theta}{\partial z} \end{cases} \quad (32)$$

where  $u$  is the wind speed and  $\theta$  is the potential temperature. The diffusion coefficient is:

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

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

$$Ri = \frac{g \frac{\partial \theta}{\partial z}}{\theta_0 \left( \frac{\partial u}{\partial z} \right)^2} \quad (34)$$

where  $g$  is the acceleration of gravity and  $\theta_0$  is a constant. The values that are used for the constants  $b$  and  $n$  are (*Girard and Delage 1990*):  $n=-2$  and  $b=5$  for  $Ri>0$  and  $n=1/2$  and  $b=20$  for  $Ri<0$ . This type of equations 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 (Girard and Delage 1990).

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  $\theta$  are  $10 \text{ ms}^{-1}$  and  $310 \text{ K}$  respectively, in every point of the domain except in the middle point where  $u$  is  $0 \text{ ms}^{-1}$  and  $\theta$  is  $250 \text{ K}$ .

The system is solved by two different methods: 1) 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 2) the method presented in this paper, with  $\beta=1/2$  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 3 iterations.

As can be seen in fig.7, where the time evolution of  $\theta$  in the middle point of the domain is shown for the first  $500000$  s, the solution obtained with the “implicit” method is noisy for time steps of  $100$  and  $1000$  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  $950000$  s to  $1000000$  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  $310 \text{ K}$  is obtained.

With the new method the simulations were performed with a time step of  $1000$  s, but the results for the new scheme are independent of the time step used (at least in the range between  $1$  to  $10000$  s). This test shows that the new method has less 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 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. 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 is 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 explicitly in time.

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$\beta$	$k \text{ (m}^2\text{s}^{-1}\text{)}$	time (s)	RMS error
1/2	1	100	9.65522E-2
1/2	1	500	1.18139E-1
1/4	1	100	1.00434E-3
1/4	1	500	4.23027E-4
1/6	1	100	3.26799E-2
1/6	1	500	4.13800E-2
1/2	10	100	6.64590E-3
1/2	10	500	7.56742E-3
1/4	10	100	2.97326E-3
1/4	10	500	3.35876E-3
1/6	10	100	1.42019E-3
1/6	10	500	1.80493E-3

Table 1 -Results with the new scheme with linear interpolation, for the case of a constant diffusion coefficient (see text for details).

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

Table II - As in table I but for the new scheme with cubic interpolation.

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

Table III - As in table I but for the implicit scheme.

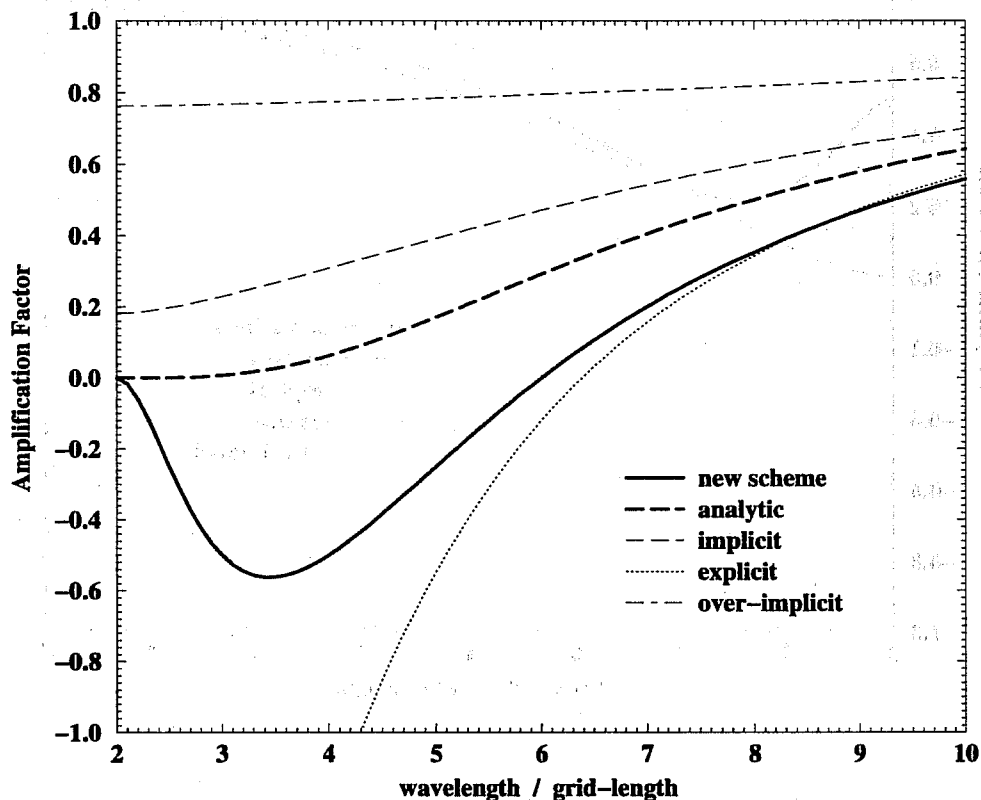


Figure 1: The amplification factor versus the wavelength divided by the grid-length, for the new, the explicit and the implicit schemes. Results obtained with  $\beta=1/2$  which corresponds (assuming  $\Delta s-\Delta x=0.5\Delta x$ ) to  $\alpha=1.12$ . Also shown is the analytic solution and an "over-implicit"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

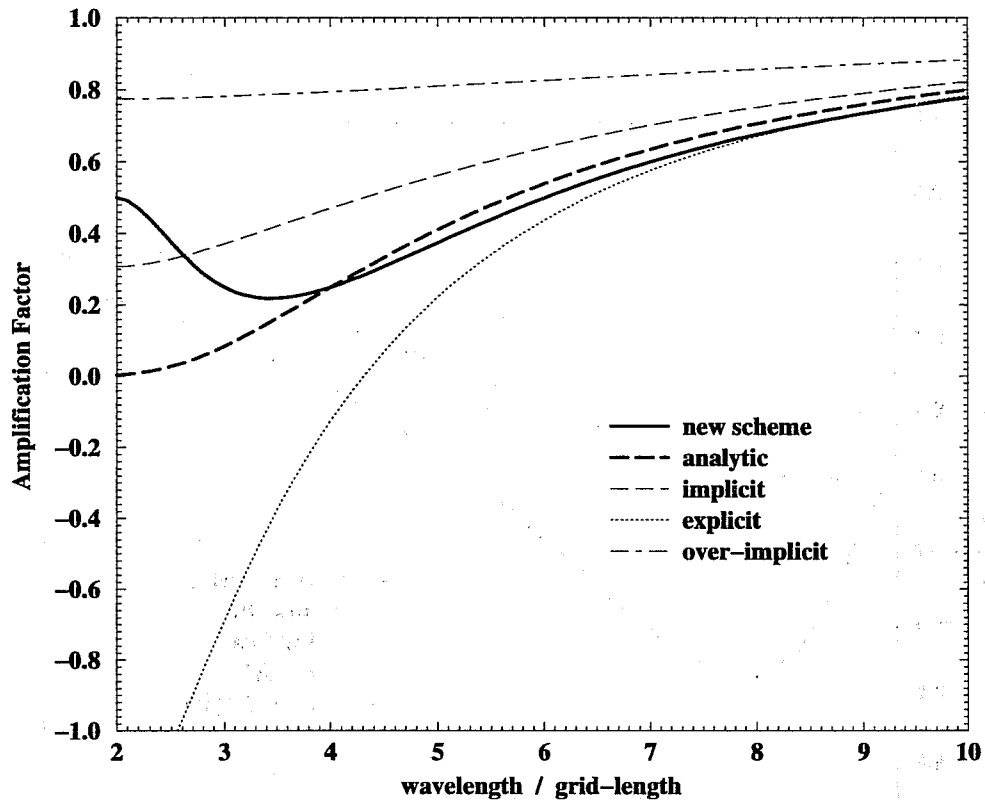


Figure 2: As in fig.1 but for  $\beta=1/4$  and  $\alpha=0.5625$ .



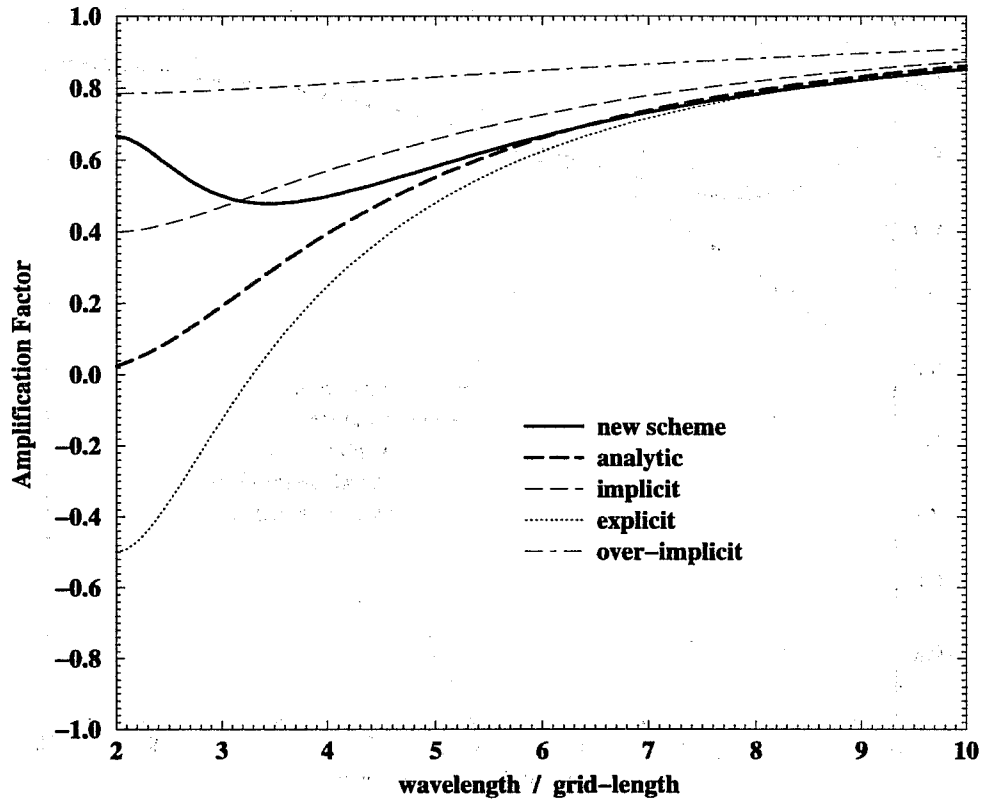


Figure 3: As in fig.1 but for  $\beta=1/6$  and  $\alpha=0.375$ .

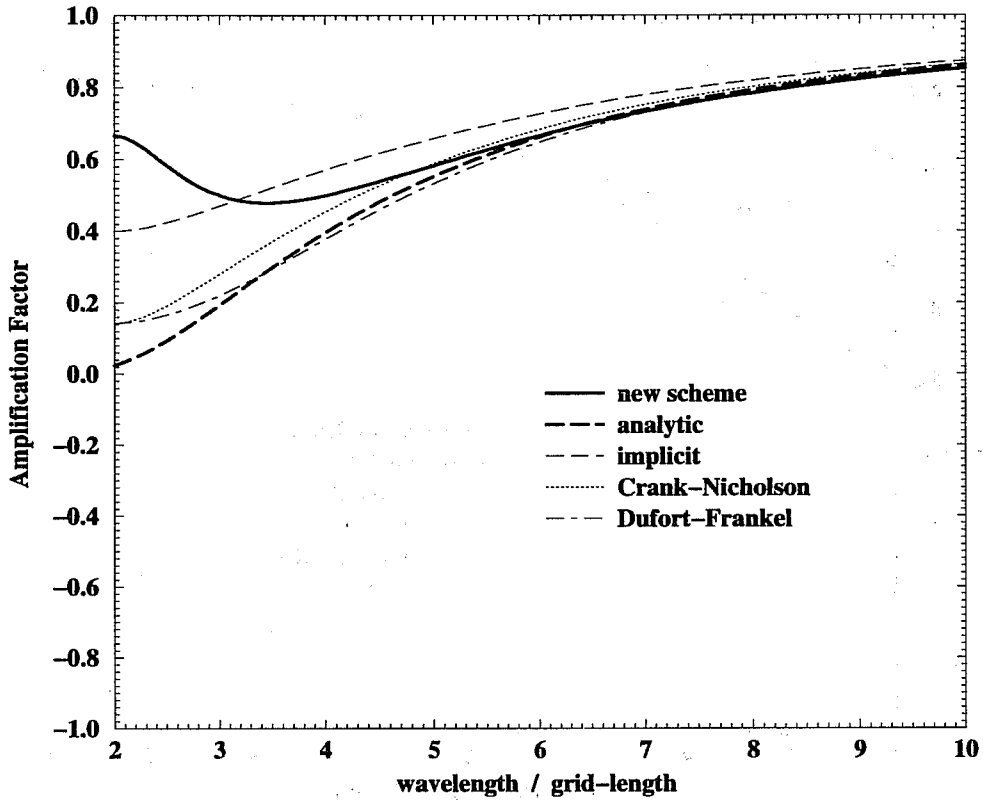


Figure 4: The amplification factor versus the wavelength divided by the grid-length, for the analytic solution, the new scheme, the implicit scheme and also for the Crank-Nicholson and the Dufort-Frankel schemes. Results obtained with  $\beta=1/6$  and  $\alpha=0.375$ .

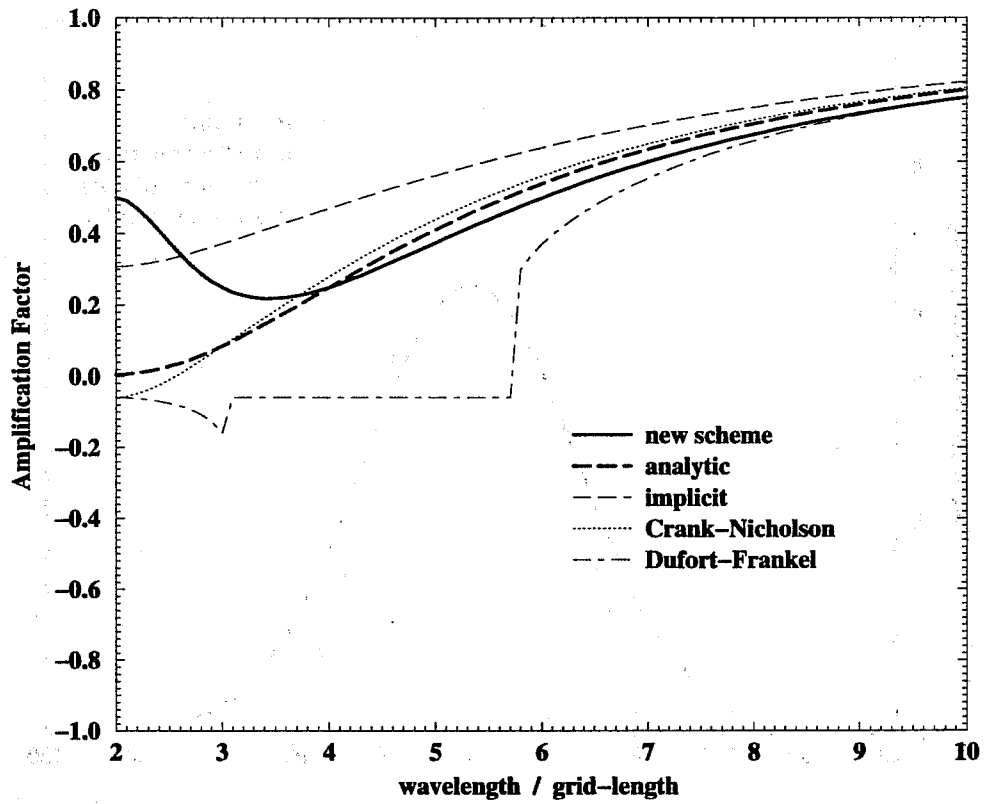


Figure 5: As in fig.4 but for  $\beta=1/4$  and  $\alpha=0.5625$ .

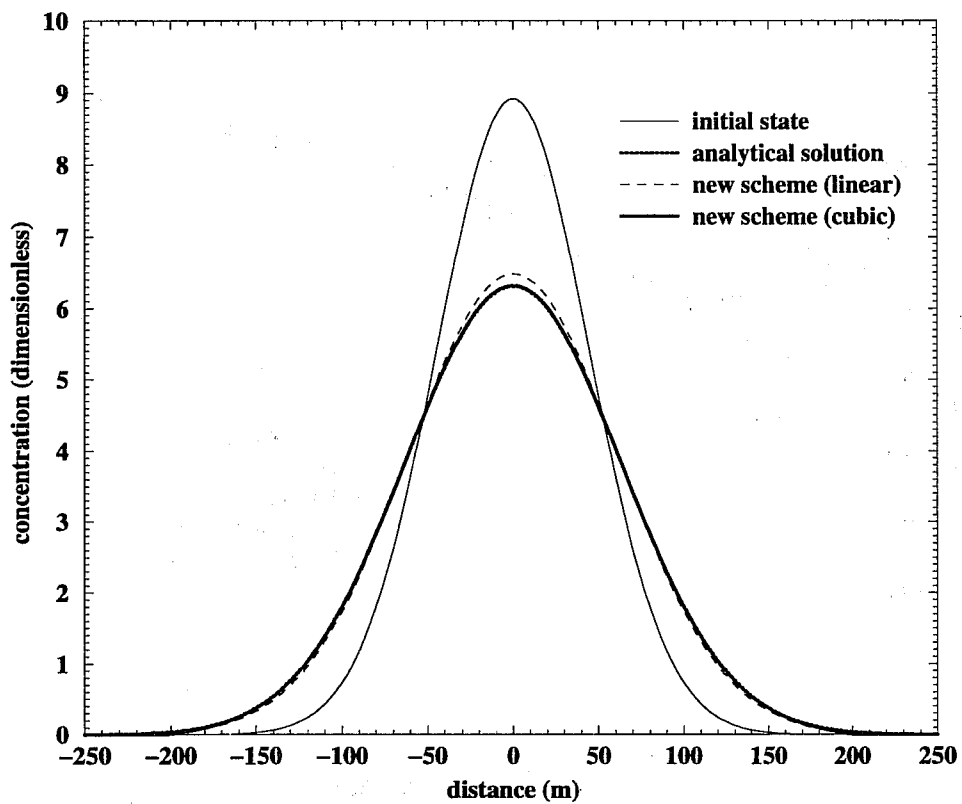


Figure 6: The initial state, the analytical solution at time  $t=200$  s, and two numerical solutions obtained with the new method 100 s after the initial state: one using linear interpolation and the other cubic interpolation.

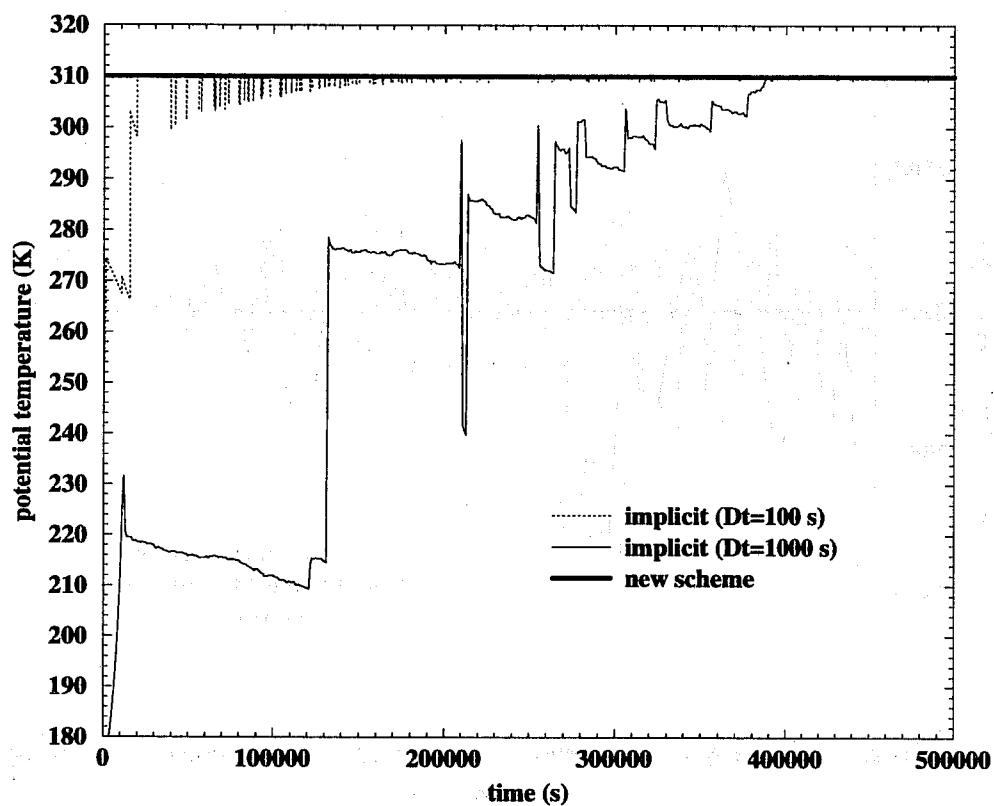


Figure 7: Time evolution of  $\theta$  in the middle point of the domain for the first 500000s, obtained with the "implicit" method (time steps of 100 and 1000 s) and with the new scheme.

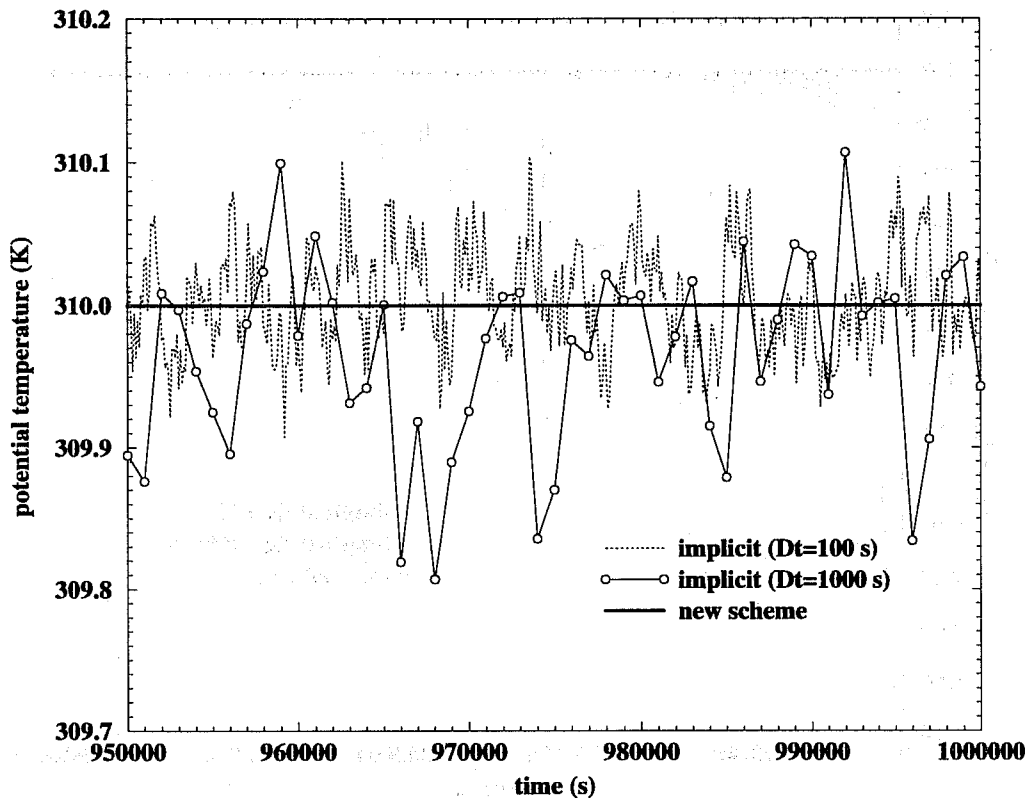


Figure 8: As in fig. 7, but for the last 50000 s of a run of 1000000 s.