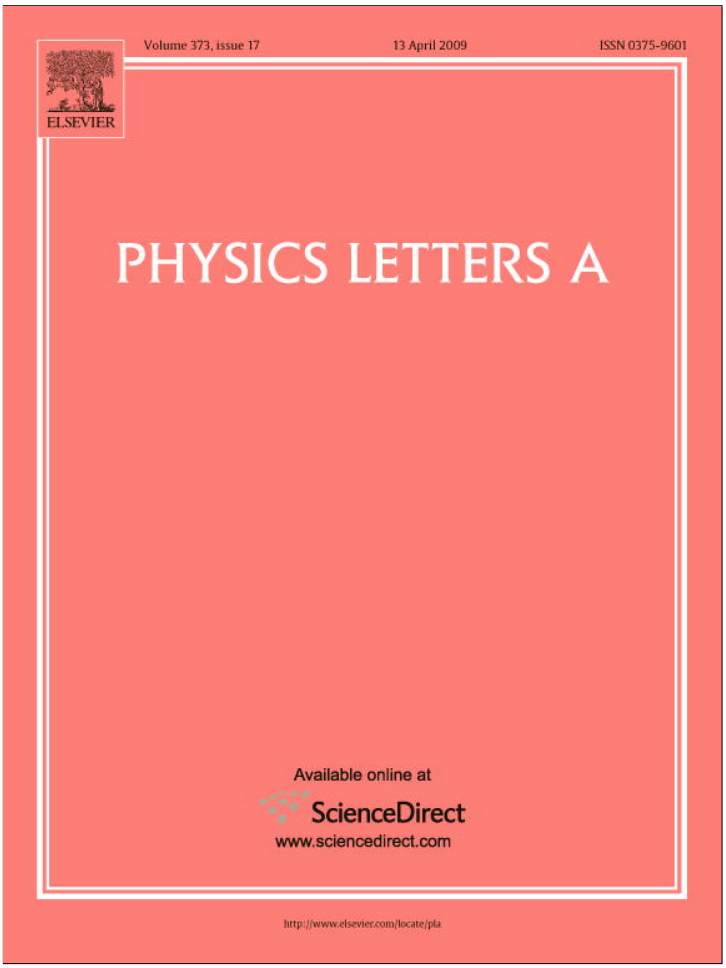

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A computationally efficient scheme for the non-linear diffusion equation

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ABSTRACT

This Letter proposes a new numerical scheme for integrating the non-linear diffusion equation. It is shown that it is linearly stable. Some tests are presented comparing this scheme to a popular decentered version of the linearized Crank–Nicholson scheme, showing that, although this scheme is slightly less accurate in treating the highly resolved waves, (i) the new scheme better treats highly non-linear systems, (ii) better handles the short waves, (iii) for a given test bed turns out to be three to four times more computationally cheap, and (iv) is easier in implementation.

1. Introduction

Most fluid mechanical systems exhibit dissipation, either due to viscosity or turbulent processes. Even when the phenomena of interest are governed by essentially inviscid processes, it is often necessary to incorporate some numerical dissipative effects in numerical models [1], for instance, to remove spurious energy accumulation at the smallest resolved scales.

In atmospheric models (numerical weather prediction, general circulation models, climate modeling), planetary boundary layer turbulence is one of the primary processes for transport of energy, momentum and moisture. The turbulence schemes are often empirical subgrid parameterizations such as, for instance, the Louis scheme [2], or the more sophisticated Turbulent Kinetic Energy (TKE) schemes (for an example see Ref. [3]). Those turbulent diffusive processes can get different forms, ranging from a simple non-linear diffusion equation to various non-linear higher-order differential operators. Since such parameterizations exhibit already a substantial modelling error in their mathematical formulation, their accuracy is of less importance than the computational efficiency.

A well-known scheme for treating the diffusion equation is the Crank–Nicholson scheme [4]. If this scheme is applied to the linear diffusion equation expressed in terms of second-order centered spatial derivatives, it relies on the inversion of a tridiagonal matrix to compute the time step. As was shown in Ref. [5], this method is problematic in the case of non-linear diffusion in the planetary boundary layer. The non-linearity is situation dependent, leading to two problems: (i) even though many algorithms for solving non-linear equations exist [6], it is very unpractical to apply them for solving the Crank–Nicholson equation in the context of atmospheric model codes, and (ii) for long time steps the system may start to exhibit artificial oscillations.

In practice, algorithmic constraints in atmospheric models often force us to invent numerical schemes for vertical diffusion that are different than the ones used for ordinary differential equations [8], nor is it possible to rely on general classes of algorithms for solving partial differential equations [9]. For this reason some atmospheric model codes, such as, for instance, the IFS code [7] apply schemes resembling the Crank–Nicholson scheme, but where the diffusion coefficients are computed explicitly. Stable solutions can be obtained by applying schemes that are decentered in time [1], i.e. so-called overimplicit schemes. These schemes need the inversion of a tridiagonal matrix, which, within the current state of operational atmospheric models may obfuscate the model code, and sometimes seriously restricts the introduction of new scientific developments. For instance, the implementation of a stable surface

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scheme within IFS numerical weather prediction model has been severely complicated by the algorithm of the vertical turbulent diffusion in the atmospheric part of the model [10].

In this Letter, we propose an alternative numerical finite-difference scheme for solving the non-linear diffusion equation. It has been put forth to address some specific needs within the above-mentioned context of atmospheric modelling. The proposed scheme in the present Letter computes the spatial derivatives of the diffusive operator in an explicit manner, but nevertheless treats the dissipated field partially in an implicit manner. As such it does not need an inversion of an off-diagonal matrix. We argue that this provides an alternative solution for the mentioned problems in the atmospheric models, but we believe that this scheme may be of interest for a more general class of applications as well.

2. The scheme

This Letter focuses on the following diffusion equation

$$\frac{\partial\psi}{\partial t} = \frac{\partial}{\partial z}\nu(\psi)\frac{\partial\psi}{\partial z}, \tag{2.1}$$

where the diffusion coefficient ν depends on the field ψ, yielding a non-linear differential operator. This equation expresses for instance the turbulent diffusion in atmospheric models, where the diffusion coefficients appear as the turbulent exchange coefficients.

A general class of integration schemes for this is

$$\frac{\psi_j^{n+1}-\psi_j^n}{\Delta t} = \xi\frac{\nu_{j+\frac12}^{n+1}(\psi_{j+1}^{n+1}-\psi_j^{n+1})-\nu_{j-\frac12}^{n+1}(\psi_j^{n+1}-\psi_{j-1}^{n+1})}{\Delta z^2} + (1-\xi)\frac{\nu_{j+\frac12}^{n}(\psi_{j+1}^{n}-\psi_j^{n})-\nu_{j-\frac12}^{n}(\psi_j^{n}-\psi_{j-1}^{n})}{\Delta z^2}, \tag{2.2}$$

where $j = 1,\dots,N$ is the index of the grid points z_j on a domain from 0 to L with $z_0 = z_N$ and with constant grid-point distance $\Delta z = z_{j+1} - z_j$. Here ψ_j^n represents a numerical approximation to $\psi(t_0 + n\Delta t, z_0 + j\Delta z)$. The coefficients $\nu_{j+\frac12}$ are evaluated on the intermediate points halfway between the grid points $j+1$ and j. The parameter ξ specifies the degree of decentering. The scheme is second-order accurate in time for $\xi = 1/2$, being the well-known Crank–Nicholson scheme [4]. Increasing ξ will increase the stability but will decrease its accuracy. In the case $\xi > 1$, this scheme is called overimplicit. For a specific application, Eq. (2.2) should be supplemented with the expressions to compute the coefficients $\nu_{j+\frac12}^{n+1}$ as a function of the values ψ_j^{n+1} and ψ_{j+1}^{n+1}.

Except in the purely explicit scheme where $\xi = 0$, the scheme in Eq. (2.2) is difficult to solve since one essentially has to solve non-linear equations. A popular trade off between both schemes is the frequently used *explicit coefficient, decentered field* (ECDF) scheme:

$$\frac{\psi_j^{n+1}-\psi_j^n}{\Delta t} = \xi\frac{\nu_{j+\frac12}^{n}(\psi_{j+1}^{n+1}-\psi_j^{n+1})-\nu_{j-\frac12}^{n}(\psi_j^{n+1}-\psi_{j-1}^{n+1})}{\Delta z^2} + (1-\xi)\frac{\nu_{j+\frac12}^{n}(\psi_{j+1}^{n}-\psi_j^{n})-\nu_{j-\frac12}^{n}(\psi_j^{n}-\psi_{j-1}^{n})}{\Delta z^2}, \tag{2.3}$$

where the diffusion coefficient ν is taken at time level n instead of time level $n+1$ in Eq. (2.2), which can then be straightforwardly computed from the available ψ_j^n. It still has a better stability than the purely explicit scheme, and the computational cost is reduced compared to the scheme in Eq. (2.2), being now mainly dominated by matrix inversions of tridiagonal systems. Cheap algorithms [1, 11] exist whose algorithmic cost scales linearly with the size N of the domain. In the present Letter, it was decided not to rely on existing numerical packages [12] but coding the scheme in FORTRAN, mimicking as much as possible the way it is done in existing atmospheric models. The matrix inversion in Eq. (2.3) has been carried out by calling the algorithm for the periodic domain as presented in the appendix of Ref. [1].

The scheme in Eq. (2.3) is popular in atmospheric models such as the European IFS model [7]. In that case it is utilized with $\xi = 1.5$ to avoid non-linear numerical instabilities [5,7]. Also in the context of atmospheric models, a stability dependent choice of the coefficient ξ was proposed in Ref. [13] and in Ref. [14], a scheme has been tested that approximates Eq. (2.2) by an iterative procedure.

In this Letter we introduce a conditionally stable scheme which shares the same computational cost of the purely explicit scheme. If ψ is a variable that, for physical reasons can never be zero (for instance, temperature expressed in Kelvin), we can compute

$$\alpha_j \equiv -\frac{1}{\Delta z^2}\frac{\nu_{j+\frac12}(\psi_{j+1}-\psi_j)-\nu_{j-\frac12}(\psi_j-\psi_{j-1})}{\psi_j}, \tag{2.4}$$

the new scheme is then

$$\psi_j^{n+1}-\psi_j^n = -\alpha_j^n\Delta t\left[\gamma\psi_j^{n+1}+(1-\gamma)\psi_j^n\right], \tag{2.5}$$

where γ is a decentering parameter in the same spirit as ξ in Eq. (2.3). Note that α has the physical meaning of a local damping coefficient.

A stability condition on γ is provided by Von Neumann's method, i.e. the amplification $\mathcal{A}$ defined by $\psi_j^{n+1} = \mathcal{A}\psi_j^n$ is computed and the stability condition is that $|\mathcal{A}| < 1$. The analysis is relevant for the damping case, i.e. $\nu > 0$ is constant. Then scheme in Eq. (2.5) becomes

$$\psi_j^{n+1}-\psi_j^n = \frac{\gamma\beta(\psi_{j+1}^n-2\psi_j^n+\psi_{j-1}^n)}{\psi_j^n}\psi_j^{n+1} + (1-\gamma)\beta\left(\psi_{j+1}^n-2\psi_j^n+\psi_{j-1}^n\right), \tag{2.6}$$

where

$$\beta = \frac{\nu\Delta t}{(\Delta z)^2} > 0.$$

For a monochromatic mode $\psi_j^n = \exp(ikz)$,

$$\psi_{j\pm1}^n = \exp(\pm ik\Delta z)\psi_j^n. \tag{2.7}$$

Plugging Eq. (2.7) into scheme (2.6) we get

$$\psi_j^{n+1} = \frac{1+2(\gamma-1)\beta(1-\cos(k\Delta z))}{1+2\gamma\beta(1-\cos(k\Delta z))}\psi_j^n.$$

It is obvious that the scheme is stable for all values of k and ν provided that $\gamma \geqslant \frac12$.

3. Numerical experiments

The reference test bed that will be considered are the simplified tests presented in Ref. [5]. In that paper, a simple non-linear damping equation

$$\frac{dX}{dt} = -\left(KX^P\right)X + S, \tag{3.1}$$

was considered with $X(t)$ a real variable depending on time t only, K and P respectively represent the degree of stiffness and non-linearity. The forcing was chosen as,

$$S(t) = 1 + \sin\left(2\pi\frac{t}{20}\right).$$

The partial differential equation

$$\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial z}\nu\frac{\partial \psi}{\partial z} + S_d, \tag{3.2}$$

effectively reduces to Eq. (3.1) if ψ a complex monochromatic one-dimensional wave of the form,

$$\psi(z,t) = X(t)e^{imz}, \tag{3.3}$$

with $X(t)$ real and where the diffusion coefficient is taken as

$$\nu(z) = C\big[\psi(z,t)\psi^*(z,t)\big]^{P/2}. \tag{3.4}$$

Here ψ^* denotes the complex conjugate of ψ, and with $C = K/m^2$ and $S_d = Se^{imz}$. As can be seen in Ref. [5], $X(t)$ never becomes zero in the tests carried out in that paper.

The diffusive part of Eq. (3.2) has been discretized by the ECDF scheme introduced in Eq. (2.3). The forcing term S_d at time $t_n = t_0 + n\Delta t$ was incorporated in the form

$$S_n = 1 + \sin\left(\frac{n\pi\,\Delta t}{10}\right) \tag{3.5}$$

by adding it at the right-hand side of Eq. (2.3). This is exactly the same form as in Ref. [5]. The diffusion coefficient is computed on the intermediate points by

$$\nu_{j+\frac{1}{2}} = C\Big[\psi^*_{j+\frac{1}{2}}\psi_{j+\frac{1}{2}}\Big]^{P/2} \tag{3.6}$$

with $\psi_{j+\frac{1}{2}} \equiv \frac{1}{2}(\psi_j + \psi_{j+1})$.

For the new scheme in Eqs. (2.4)–(2.5) there is a subtlety to address in the way the forcing S_d is coupled. In fact two options have been studied.

The first one is

$$\psi_j^{n+1} = \frac{1-\alpha_j^n\Delta t(1-\gamma)}{1+\alpha_j^n\Delta t\gamma}\psi_j^n + \frac{\Delta t}{1+\overline{\alpha^n}\Delta t\gamma}S_n, \tag{3.7}$$

which is obtained by adding the term in Eq. (3.5) to the right-hand side of Eq. (2.5), but where, in the last term in Eq. (3.7), the α_j^n has been substituted by $\overline{\alpha^n}$, being the average of α_j^n,

$$\overline{\alpha^n} = \frac{1}{N}\sum_{j=1}^{N}\alpha_j^n. \tag{3.8}$$

This scheme will be referred to as the NEW scheme. The substitution of α_j^n by $\overline{\alpha^n}$ is an important detail. When this was not done, and when the model was integrated with a very high spatial resolution, it was found that numerical noise entering through α_j^n in the denominator of the forcing term, started to force the numerical solution in a substantial manner, amplified by a non-linear feedback between the forcing and spurious oscillations of the diffusion.

Secondly, a scheme with two fractional steps [1] has been considered with the forcing coupled after the diffusion,

$$\begin{aligned}\tilde{\psi}_j - \psi_j^n &= -\alpha_j^n\Delta t\big[\gamma\tilde{\psi}_j + (1-\gamma)\psi_j^n\big],\\ \psi_j^{n+1} - \tilde{\psi}_j &= \Delta t S_n.\end{aligned} \tag{3.9}$$

This is the way different physical processes are treated in the IFS model [7]. No problems have been observed with this scheme in the setup presented here.

Note that no matrix inversion is needed in Eqs. (3.7) and (3.9). The results of the tests will be only presented for the scheme

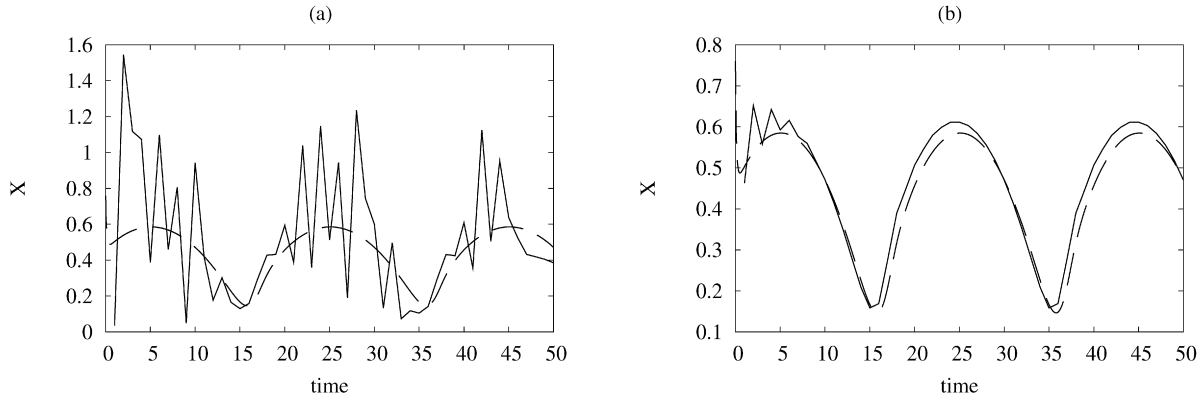

Fig. 1. The amplitude X as a function of time of the NEW scheme with $K = 10$, $P = 2$, $N = 10$ and (a) $\gamma = 0.5$ and (b) $\gamma = 1.5$, indicated by the solid line. We have used a resolution $\Delta z = 1$ and $\Delta t = 1$. The dashed line represents the reference solution obtained by the centered ECDF scheme with high resolution $\Delta t = 0.01$ and $\Delta z = 0.1$, $N = 100$ with $\xi = 0.5$.

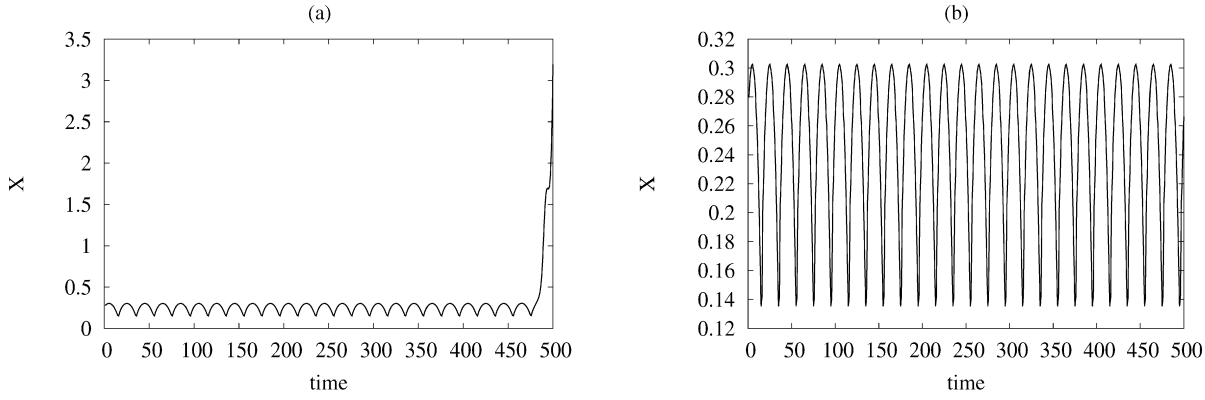

Fig. 2. The amplitude X on a domain with $N = 10$, for (a) ECDF with $K = 1000$, $P = 4$, $\xi = 6.0$, and (b) NEW with $K = 1000$, $P = 4$, $\gamma = 4.0$.

NEW as introduced in Eq. (3.7). This NEW scheme and the ECDF scheme have been tested taking as initial condition a periodic field $\psi(z, t = 0)$ of the form introduced in Eq. (3.3), with wave length $L = N\Delta z$, and $m = \frac{2\pi}{N\Delta z}$. By restricting the tests to periodic fields, the problem of the boundary conditions [15] is not studied in the present Letter. The numerical solution of the scheme (3.7) should then be comparable to the ones obtained with (3.8) in Ref. [5]. We investigated the numerical behavior of the methods in the particular situations: $K = 10$ (non-stiff), $K = 1000$ (stiff), and the non-linearity ranging from $P = 1$ (mildly non-linear) to $P = 4$ (strongly non-linear).

We start with an illustration of the effect of the decentering parameter γ in Eq. (2.5). We consider a resolution $\Delta z = 1$ and $\Delta t = 1$. In Fig. 1 it can be seen that the use of the scheme in Eq. (2.5) with $K = 10$, $P = 2$, $N = 10$ and $\gamma = 0.5$ leads to spurious solutions, but that, by taking $\gamma = 1.5$, they are removed. This can be compared to a reference solution, also indicated in Fig. 1 that has been obtained by the centered ECDF scheme with $\xi = 0.5$, with a high resolution of $\Delta t = 0.01$ and $\Delta z = 0.1$, and with $N = 100$, giving a good estimate of the exact solution.

Table 1
The chosen values of the parameters ξ for the ECDF scheme and γ for the NEW scheme to remove the oscillation for different values of P and K for $N = 1$, 10, 100.

		$K = 10$				$K = 1000$			
		$P = 1$	$P = 2$	$P = 3$	$P = 4$	$P = 1$	$P = 2$	$P = 3$	$P = 4$
$N = 4$	ξ	1.0	NaN	NaN	NaN	1.5	NaN	NaN	NaN
	γ	1.0	1.5	2.0	2.5	1.5	2.0	3.0	4.0
$N = 10$	ξ	1.0	1.5	2.0	NaN	1.5	2.0	3.0	NaN
	γ	1.5	1.5	2.0	2.5	1.5	2.0	3.0	4.0
$N = 100$	ξ	1.0	1.5	2.0	NaN	1.5	3.0	4.0	NaN
	γ	2.5	2.5	4.0	5.0	2.0	3.0	5.0	6.0

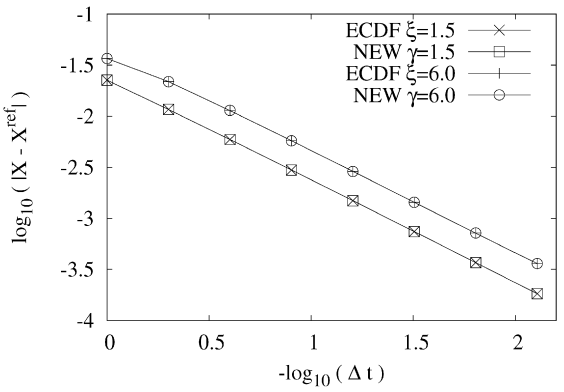

Fig. 3. Accuracy tests for NEW and the ECDF schemes for $P = 2$, $K = 10$ and $N = 10$. The reference is a run with $\Delta t = 0.0001$, $\Delta z = 1$, $\xi = 1/2$.

In the case $P = 4$, $K = 1000$, the solution of the ECDF scheme started to grow after 450 time steps, as can be seen from Fig. 2a. As shown in Fig. 2b this behavior did not occur in the NEW scheme. The same problem occurred for $N = 4$ and $P = 2, 3, 4$. Increasing the decentering ξ did not cure the problem. It only made it stable for a longer time period but eventually this type of numerical instability did show up in the integration. This is indicated in Table 1 by NaN (Not a Number). In other words, for sufficiently high non-linearity, the ECDF scheme exhibits this kind of unstable behavior. For $N = 4$ and $N = 10$ the choices of the decentering parameters for the ECDF and the NEW scheme coincide, except (i) in the case $P = 1$, $K = 10$, where the NEW scheme with $\gamma = 1.0$ started to show small oscillations after 250 time steps, and (ii) the unstable cases for the ECDF scheme indicated by NaN, where the integration showed an instability of the kind in Fig. 2a. If the mode becomes more resolved, i.e. considering $N = 100$, higher decentering values are needed for γ of the NEW scheme in order to remove the spurious oscillations.

Next, we analyze the effect of the parameter values on the accuracy of the method. As in Ref. [5] we consider the time interval $t \in [0, 50]$. A reference solution at the endpoint $t_{\text{end}} = 50$ is obtained by considering the ECDF scheme with very small time step $\Delta t = 0.0001$, taking $\Delta z = 1$, and with $\xi = 1/2$ (making it second-order accurate), yielding the field X^{ref}. The error at t_{end} is taken as $|X(t_{\text{end}}) - X^{\text{ref}}(t_{\text{end}})|$. Fig. 3 shows a log–log plot of the error at t_{end} as a function of $\Delta t = 1/2^j$ $(j = 0, 1, \ldots, 7)$ for $P = 2$, $K = 10$, $N = 10$ and for decentering values 1.5 and 6.0. The NEW scheme has exactly the same accuracy curve as the ECDF scheme.

Finally, the computational efficiency of both schemes were compared. This was estimated by running the scheme with 1000 time steps, and for values of N ranging from 100 to 1000. The measurement of the cpu time in both ECDF and NEW was, in the code, restricted to the operations needed to solve Eqs. (2.3) and (3.7) respectively. In Fig. 4a the average cpu time was taken of 2000 integrations. It can be seen from this figure that in both cases the increase in computational cost grows linearly. Fig. 4b shows the ratio of the $\text{cpu}_{\text{ECDF}}/\text{cpu}_{\text{NEW}}$. This shows, that for this test, the

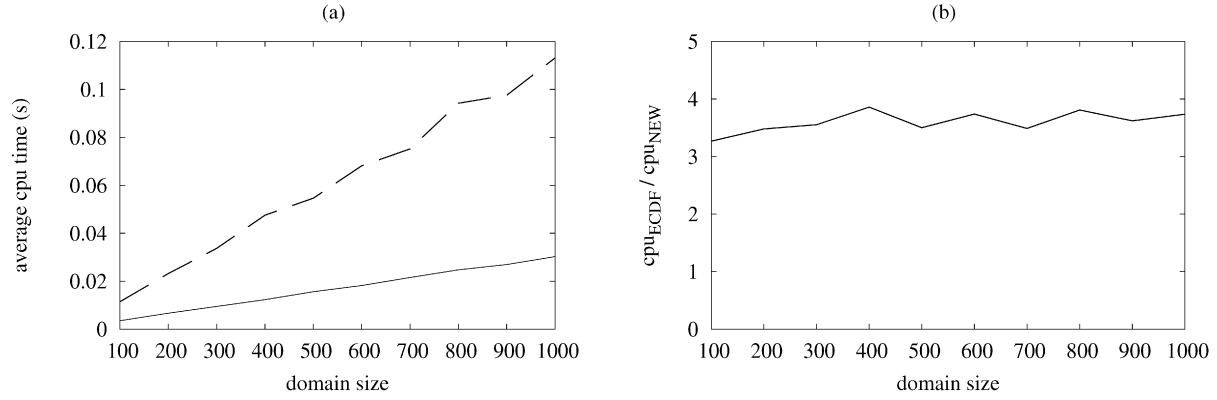

Fig. 4. The cpu time (a) in both NEW scheme (solid line) and the ECDF scheme (dashed), for domain sizes ranging from 100 to 1000 grid points, and (b) the ratio of the cpu time of the ECDF scheme over the cpu time of the NEW scheme.

NEW scheme is about three to four times cheaper than the ECDF scheme.

4. Discussion

This Letter proposed an alternative scheme for solving the non-linear diffusion equation. For well-resolved modes it has been shown to be equivalent to a scheme that is popular in the current atmospheric models. For short waves and for strongly non-linear systems, it has been shown to behave better. In the presented tests, it turned out to be three to four times as computationally efficient as the reference scheme.

On the other hand, for the long waves it has also been shown that it needs to be applied with more decentering to control the spurious oscillations. We think two options are worth studying to improve this: (i) introducing a protection against a potential division by zero in Eq. (2.4) and (ii) applying some numerical filtering to control the $2\Delta x$ mode. The study of this lies beyond the domain of application of the present study and thus beyond the scope of the present Letter.

This Letter is restricted to a diffusion scheme with second-order finite difference approximation for the derivatives, in which case the matrix to be inverted is tridiagonal. For a scheme using higher-order finite difference derivatives, the matrix inversion would become even more computationally expensive. By avoiding the inversion, the proposed new scheme may pay off even more in that case.

Besides vertical turbulent diffusion in atmospheric models, we believe that the proposed scheme may also be useful in other contexts. In Ref. [16] it is described how in the IFS model [7], the computation of the derivatives in the diffusive parameterisation is restricted to time level t for algorithmic reasons coming from the fact that the derivatives are computed with Galerkin spectral methods. This currently complicates the development of three-dimensional turbulent diffusion parameterisation schemes that can be called within operational models running with long time steps. Indeed, in this model the derivatives of dissipative non-linear differential operators of such schemes are necessarily explicit. If the presently proposed scheme could be extended to such operators, it would be worthwhile to investigate whether this problem could be solved by dividing the field at time level t and multiplying by the field at time level $t + \Delta t$ to construct the implicit term.

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