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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.

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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

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

where $j = 1,\ldots,N$ 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 $\nu_{j+\frac{1}{2}}$ 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 $\nu_{j+\frac{1}{2}}^{n+1}$ 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:

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

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

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

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 $\gamma \geqslant \frac{1}{2}$.

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,

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

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