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Accuracy and Stability of the Discretised Isopycnal-Mixing Equation

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Abstract—Coarse-grid ocean models parameterise the effects of mesoscale eddies by means of a mixing operator which diffuses tracers along surfaces of constant potential density, called isopycnals. We establish the consistency conditions, the spatio-temporal accuracy error and the computational stability conditions for the small-slope isopycnal mixing operator.

Keywords—Ocean model, Isopycnal diffusion, Computational stability and accuracy.

1. INTRODUCTION

Ocean General Circulation Models (OGCMs) with coarse horizontal resolution cannot resolve explicitly the mesoscale eddies. It is generally believed that mesoscale eddies cause tracers, such as temperature or salinity, to mix predominantly along surfaces of constant potential density—called isopycnals—rather than along horizontal surfaces [1]. This is why Redi [1] suggested that a mixing operator leading to diffusion along isopycnals be used. The latter was impractical for OGCM, so Cox [2] introduced a simplified form, obtained by taking chiefly into account the smallness of the slope of the isopycnals (α is about 10^{-3}).

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Numerical properties of accuracy and stability of the isopycnal mixing scheme of [2] are explored in this paper. In Section 2, the isopycnal diffusion operator and its discretisation are briefly described. In Section 3, the accuracy of the scheme on a nonuniform vertical grid is assessed. In Section 4, the numerical behaviour of the spatial discretisation is investigated and stability conditions for explicit and semi-implicit schemes are derived. Finally, conclusions are drawn in Section 5.

2. ISOPYCNAL MIXING FORMULATION

As the isopycnal diffusion operator of Cox [2], by contrast to Redi's, does not contain any horizontal cross-derivatives, the present discussion may be carried out in a single vertical plane without any loss of generality. Therefore, only two-dimensional operators, concerning the vertical and one horizontal direction, will be dealt with below.

2.1. Small-Slope Isopycnal Diffusion Operator

Let t, x, and z represent time, the horizontal coordinate and the vertical coordinate—increasing upward, respectively. Taking solely into account diffusion along surfaces of constant potential density ρ, the concentration C of a passive tracer obeys the following partial differential equation expressed in Cartesian coordinates:

$$\frac{\partial C}{\partial t} = D, \tag{1}$$

where D represents the isopycnal diffusion operator of [2],

$$D = \underbrace{\frac{\partial}{\partial x}\left(\kappa \frac{\partial C}{\partial x}\right)}_{D^{-}} + \underbrace{\frac{\partial}{\partial x}\left(\kappa\alpha \frac{\partial C}{\partial z}\right) + \frac{\partial}{\partial z}\left(\kappa\alpha \frac{\partial C}{\partial x}\right)}_{D^{\times}} + \underbrace{\frac{\partial}{\partial z}\left(\kappa\alpha^2 \frac{\partial C}{\partial z}\right)}_{D^{|}}, \tag{2}$$

where κ is the along-isopycnal diffusivity and $\alpha = -(\frac{\partial \rho}{\partial x})/(\frac{\partial \rho}{\partial z})$ denotes the slope of isopycnal lines. For convenience, some useful conventions are introduced to identify the different components of the isopycnal diffusion operator: $D^{\times}$, $D^{|}$, and D^{-} refer to the parts of D that are linear in the slope (x-z derivative), quadratic in the slope (z-z derivative), and independent of the slope (x-x derivative), respectively.

2.2. Discretisation

The spatial discretisation of [2] which is implemented in the widely used Geophysical Fluids Dynamics Laboratory (GFDL) model [3] is described below. Integer labels i, k, and n are associated with the horizontal, the vertical, and the temporal discretisations, respectively. So, $a^n_{i,k}$ represents the value of a variable "a" discretised at position (i, k) (Figure 1) and at time $t = n\Delta t$, where Δt is the time step. The horizontal grid spacing Δx is assumed constant, while the height of the grid box Δz_k can vary along the vertical (Figure 1). This assumption is appropriate since, in OGCMs, the vertical resolution varies much more rapidly than the horizontal resolution. It is convenient to use the following discrete difference and average operators:

$$(\delta_x a_{i,k}, \delta_z a_{i,k}) = \left(\frac{a_{i+1/2,k} - a_{i-1/2,k}}{\Delta x}, \frac{a_{i,k+1/2} - a_{i,k-1/2}}{\Delta z_k}\right), \tag{3a}$$

$$\overline{a_{i,k}}^{x,z} = \frac{a_{i+1/2,k+1/2} + a_{i-1/2,k+1/2} + a_{i-1/2,k-1/2} + a_{i+1/2,k-1/2}}{4}. \tag{3b}$$

With the above notations, the discretised form $D_{i,k}$ of the continuous isopycnal diffusion operator D reads

$$D_{i,k} = \delta_x\left(\kappa\delta_x C_{i,k} + \kappa\alpha_{i,k}\delta_z\overline{C_{i,k}}^{x,z}\right) + \delta_z\left(\kappa\alpha^2_{i,k}\delta_z C_{i,k} + \kappa\alpha_{i,k}\delta_x\overline{C_{i,k}}^{x,z}\right). \tag{4}$$

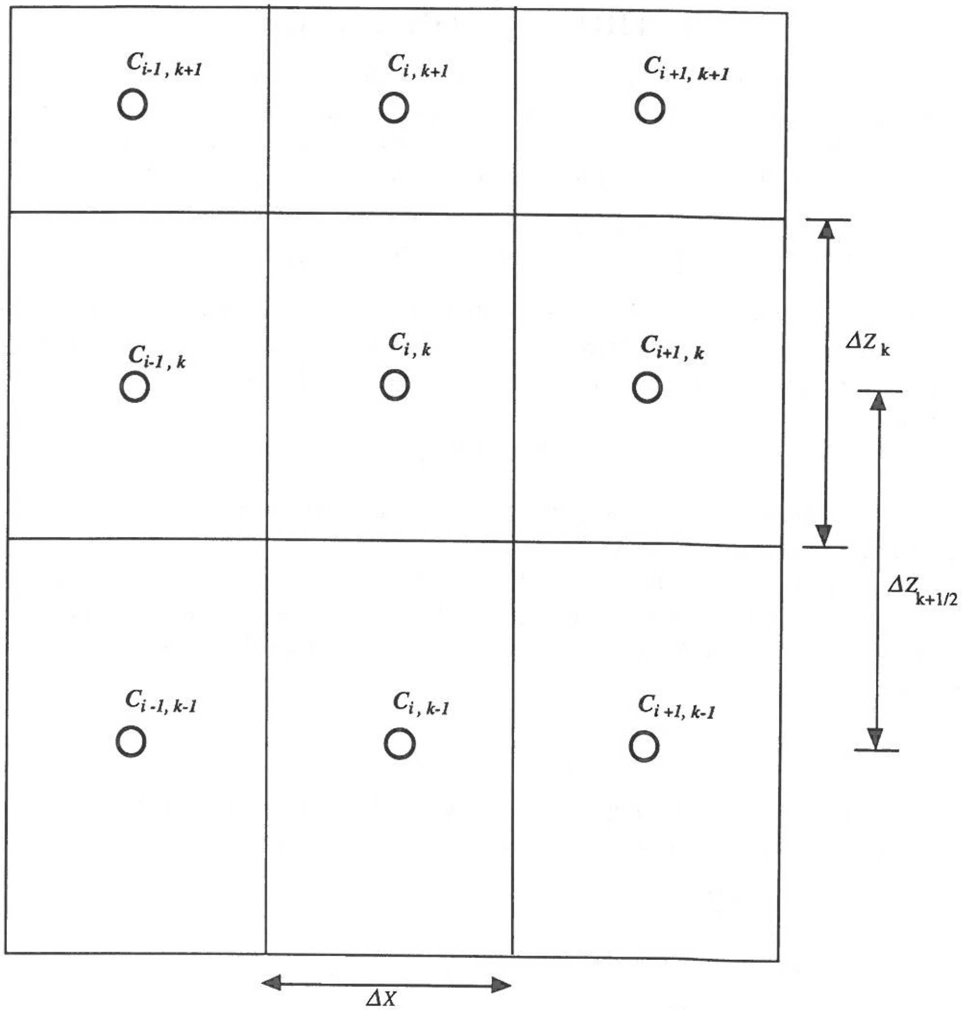


Figure 1. Numerical grid in the vertical plane. Tracer points are represented by circles.

The isopycnal slope is defined so as to guarantee that, if C were a linear function of the density, no isopycnal diffusion would occur, i.e.,

$$\left(\alpha_{i+1/2,k}, \alpha_{i,k+1/2}\right) = -\left(\frac{\delta_x \rho_{i,k}}{\delta_z \overline{\rho_{i,k}}^{x,z}}, \frac{\delta_x \overline{\rho_{i,k}}^{x,z}}{\delta_z \rho_{i,k}}\right). \tag{5}$$

For consistency with the small-slope approximation and computational stability, Cox [2] recommended to limit the slope computed according to (5) to an appropriate threshold, typically 10^{-2}.

The time stepping considered here is that of the CLIO (Coupled Large-scale Ice-Ocean) model developed at Louvain-la-Neuve (see [4,5]), which is somewhat different from the leap-frog approach of the GFDL model [3]. Accordingly, (1) is discretised as

$$\frac{C_{i,k}^{n+1} - C_{i,k}^{n}}{\Delta t} = \left(D_{i,k}^{\times}\right)^n + \left(D_{i,k}^{-}\right)^n + (1-\mu)\left(D_{i,k}^{|}\right)^n + \mu\left(D_{i,k}^{|}\right)^{n+1}, \tag{6}$$

where $\mu \in [0,1]$ is the level of implicitness of the vertical derivatives. The need for a semi-implicit resolution of $D_{i,k}^{|}$ is related to the fine vertical resolution and the magnitude of the vertical diffusivity $\kappa\alpha^2$ as discussed in Section 5.

3. TRUNCATION ERROR

In this section, we determine the spatio-temporal accuracy of the numerical scheme. We assume variable Δz and constant Δx, which is a good approximation in OGCMs. The Taylor expansion of D around point (i,k) yields the spatial truncation error ε_s of the scheme which represents the difference between the discrete operator $D_{i,k}$ and the continuous operator D:

$$\varepsilon_s = \kappa \left(\frac{\Delta z_{k+1/2} + \Delta z_{k-1/2}}{2\Delta z_k} - 1 \right) \left(\alpha^2 \frac{\partial^2 C}{\partial z^2} + \alpha \frac{\partial^2 C}{\partial z \partial x} \right) + O\left(\Delta x, \Delta z_k\right). \tag{7}$$

These terms of the error are, respectively, related to the discretisation of the vertical diffusive operator $D^{|}$ and the crossed-derivative operator $D^{\times}$. As a result of the nonuniformity of the vertical grid size, the scheme appears inconsistent (ε_s of order zero) unless the vertical grid spacing verifies

$$\Delta z_k = \frac{\Delta z_{k+1/2} + \Delta z_{k-1/2}}{2}. \tag{8}$$

For example, the above condition is verified for a vertical grid where grid box boundaries are placed at an equal distance to the adjacent tracer points.

When the vertical grid is defined according to (8), $D_{i,k}$ becomes consistent and first-order accurate in space. In order to avoid working with lengthy expressions, the isopycnal diffusivity κ and the isopycnal slope α will be taken constant for the rest of the paper. Then, the spatial truncation error reads

$$\varepsilon_s = \left(\Delta z_{k+1/2} - \Delta z_{k-1/2}\right) \left(\frac{\kappa\alpha^2}{3} \frac{\partial^3 C}{\partial z^3} + \frac{3\kappa\alpha}{4} \frac{\partial^3 C}{\partial z^2 \partial x} \right) + O\left(\Delta x^2, \Delta z_k \Delta z_{k\pm 1/2}, \Delta z_k^2\right). \tag{9}$$

Although constant vertical grid spacing is rarely used in OGCMs, it may be worth stressing that the numerical scheme becomes second-order accurate in space on such a numerical lattice

$$\begin{aligned} \varepsilon_s = {} & \frac{\kappa}{12} \left(\Delta x^2 \frac{\partial^4 C}{\partial x^4} + \alpha^2 \Delta z^2 \frac{\partial^4 C}{\partial z^4} \right) \\ & + \frac{\kappa\alpha}{3} \left(\Delta x^2 \frac{\partial^4 C}{\partial x^3 \partial z} + \Delta z^2 \frac{\partial^4 C}{\partial z^3 \partial z} \right) + O\left(\Delta x^3, \Delta z^3, \Delta x^2 \Delta z, \Delta x \Delta z^2\right). \end{aligned} \tag{10}$$

The latter error involves terms of a diffusive nature (even-order derivatives) and of a dispersive nature (odd-order derivatives). The dispersive terms, which are linear in α (i.e., associated with $D^{\times}_{i,k}$), are responsible for the nonmonotonic behaviour of the numerical isopycnal diffusion operator, as pointed out in [6,7].

By carrying out a Taylor expansion in time of (6), we obtain the following temporal truncation error for the scheme:

$$\varepsilon_T = \Delta t \left(\frac{1 \partial^2 C}{2 \partial t^2} + (\mu - 1) \frac{\partial D^{|}_{i,k}}{\partial t} \right) + O\left(\Delta t^2\right). \tag{11}$$

By virtue of (1), for constant κ and α, we have

$$\frac{\partial^m}{\partial t^m} = \kappa^m \left(\frac{\partial}{\partial x} + \alpha \frac{\partial}{\partial z} \right)^{2m}. \tag{12}$$

Substituting (12) into (11) yields the temporal truncation error in terms of spatial derivatives only. By examining the term in fourth-order horizontal derivative (i.e., $1/2\kappa^2 \Delta t \frac{\partial^4 C}{\partial x^4}$) which does not vanish systematically, it is readily seen that for $\alpha \neq \infty$, the scheme is only first-order accurate in time, whatever the value of μ. This is easily understood, since the first term of the error rewritten as $1/2 \frac{\partial D_{i,k}}{\partial t}$ cannot compensate the second term of the error which involves solely the vertical component $D^{|}$ of the operator D. In the particular case $\alpha = \infty$, the operator D degenerates to pure vertical diffusion and the value $\mu = 1/2$ leads to a scheme which is second-order accurate in time (i.e., [7]).

4. VON NEUMANN ANALYSIS

In this section, we employ the Von Neumann method [7] to explore the properties of the spatial discretisation and provide the necessary stability conditions of the diffusion equations (1),(2) with the operator D discretised according to (3)–(5). In order to perform this *linear* analysis, it is necessary to assume that α, κ, Δx, and Δz are constant.

4.1. Properties of the Spatial Dicretisation

In a periodic or infinite domain and under the assumptions above, the solution of (1) can be expressed as a sum of waves periodic in space with amplitude λ and wave numbers m_x and m_z:

$$C(x,z,t) = \lambda(t) \exp\left[I(m_x x + m_z z)\right], \qquad \text{where } I = \sqrt{-1}. \tag{13}$$

Substituting (13) into (1) yields

$$\frac{d\lambda}{dt} + \omega\lambda = 0, \tag{14}$$

where the damping coefficient ω is given by the dispersion equation

$$\omega = \kappa(m_x + \alpha m_z)^2. \tag{15}$$

It is readily shown that the solution of the differential equation (14) is

$$\lambda(t) = \lambda(0)\exp[-\omega t], \tag{16}$$

which means that the wave amplitude decays exponentially in time ($\omega \geq 0$). As the e-folding time scale ω^{-1} is quadratic in the wave numbers, the diffusive operator D tends to leave the long wave modes unaffected and strongly damps short waves except the modes verifying $\alpha = -m_x/m_z = -(\frac{\partial C}{\partial x})/(\frac{\partial C}{\partial z})$ (i.e., modes such that the slope of concentration lines equals the slope of isopycnals) (Figure 2a). This is natural, since isopycnal diffusion should not affect a tracer homogeneous along isopycnals.

In analogy with the continuous case, we consider semidiscrete periodic solutions

$$C_{i,k} = \hat{\lambda}(t)\exp\left[I(\theta_x i + \theta_z k)\right], \tag{17}$$

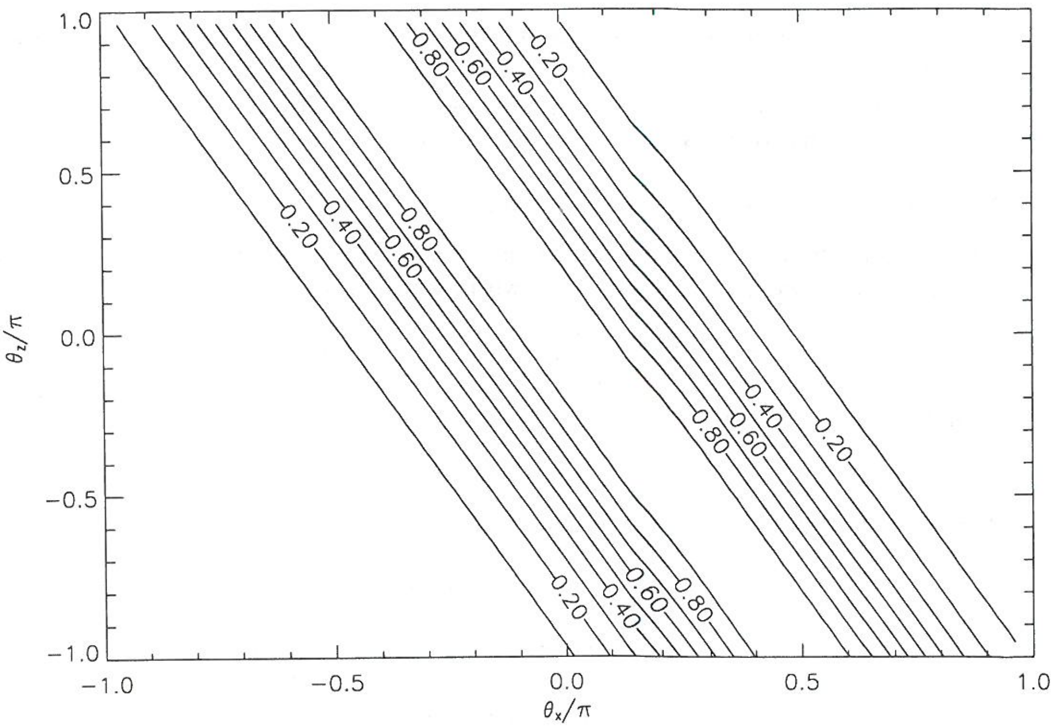
where the discrete wave numbers θ_x and θ_z are related to m_x and m_z by $-\pi \leq \theta_x = m_x\Delta x \leq \pi$ and $-\pi \leq \theta_z = m_z \Delta z \leq \pi$. By discretising the right-hand side of (1) with (4) and by introducing (17) into this semidiscrete equation, we obtain a differential equation which has the following solution for the amplitude of the discrete wave solution:

$$\hat{\lambda}(t) = \hat{\lambda}(0)\exp[-\hat{\omega} t]. \tag{18}$$

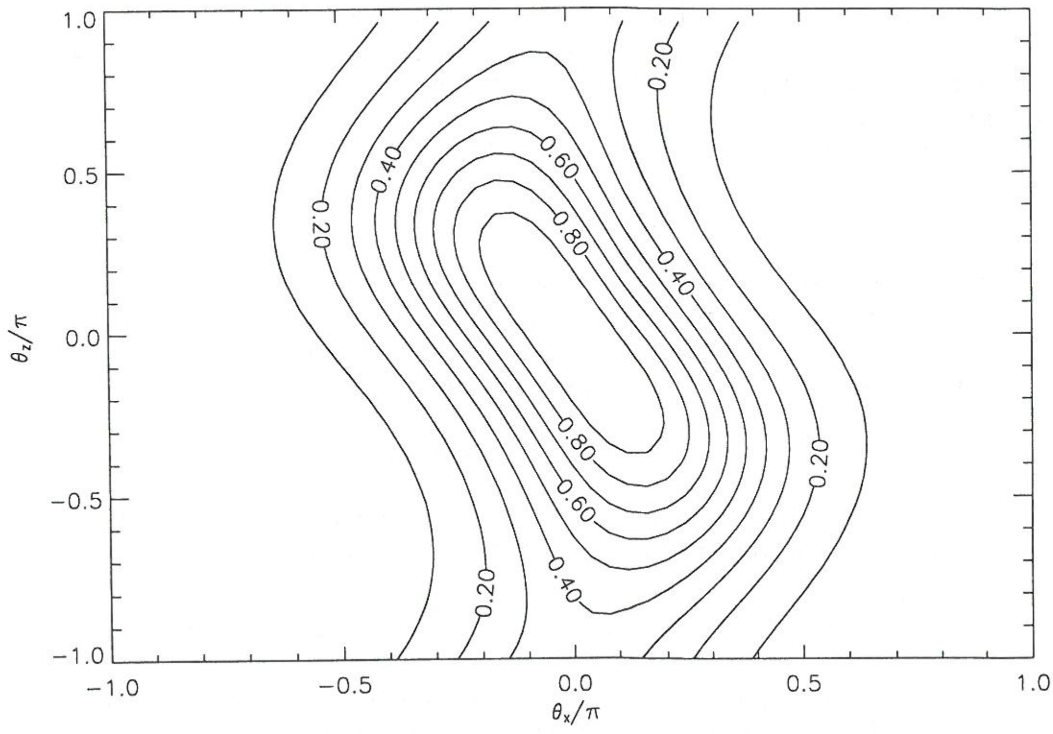
The damping coefficient $\hat{\omega}$ for the discrete scheme is expressed in terms of the grid slope ratio r which is the ratio of the isopycnal slope to the aspect ratio of the grid

$$\frac{\Delta x^2 \hat{\omega}}{\kappa} = 2(1-\cos\theta_x) + 2r^2(1-\cos\theta_z) + 2r\sin\theta_x\sin\theta_z, \qquad \text{with } r = \frac{\alpha\Delta x}{\Delta z}. \tag{19}$$

In order to explore the properties of the spatial discretisation, it is very instructive to compare the behaviour of the continuous (15),(16) and discrete (18),(19) wave amplitudes. As shown in Figure 2, the discrete operator $D_{i,k}$ provides a numerical treatment of long waves quite similar to the continuous operator D. Two modes are of special interest: the "infinite" mode $(\theta_x, \theta_z) = (0,0)$ and the "computational" or "checkerboard" mode $(|\theta_x|, |\theta_z|) = (\pi, \pi)$ associated, respectively, with the infinite wave length and the shortest wave length $(2\Delta x, 2\Delta z)$ resolved by the numerical



(a) Function $\lambda(t)$ for the continuous scheme.



(b) Function $\hat{\lambda}(t)$ for the discrete scheme.

Figure 2. Parameters $\kappa/\Delta x^2 = 0.01$ and $r = 0.5$ are used.

grid. As illustrated in Figure 2b, the operator $D_{i,k}$ does not affect the infinite mode and efficiently damps the poorly represented short waves.

4.2. Linear Stability Analysis

The Von Neumann necessary conditions for computational stability require that modes of form (18) cannot grow in time. These conditions are obtained by imposing that the module of the temporal amplification factor $G = \lambda_{i,k}^{n+1}/\lambda_{i,k}^{n}$ remains smaller than or equal to 1 for all modes (θ_x, θ_z). For the discrete scheme (4)–(6), the amplification factor G is expressed as follows:

$$G = \frac{1 - 2d(1-\cos\theta_x) - 2\,dr^2(1-\cos\theta_z)(1-\mu) - 2\,dr\sin\theta_z\sin\theta_x}{1 + 2\,dr^2(1-\cos\theta_z)\mu}, \qquad \text{where } d = \frac{\kappa\Delta t}{\Delta x^2}. \tag{20}$$

The stability conditions $G \leq 1$ and $G \geq -1$, are therefore, equivalent to the following inequalities where $\gamma = 1 - 2\mu \in [-1, 1]$:

$$F_1 = -2d(1-\cos\theta_x) - 2\,dr^2(1-\cos\theta_z) - 2\,dr\sin\theta_z\sin\theta_x \leq 0, \tag{21}$$

$$F_2 = 2 - 2d(1-\cos\theta_x) - 2\gamma\,dr^2(1-\cos\theta_z) - 2\,dr\sin\theta_z\sin\theta_x \geq 0. \tag{22}$$

The function F_1 reaches its extreme values for

$$\frac{\partial F_1}{\partial\theta_x} = 0 \rightarrow \sin\theta_x + r\sin\theta_z\cos\theta_x = 0, \tag{23}$$

$$\frac{\partial F_1}{\partial\theta_z} = 0 \rightarrow r\sin\theta_z + \sin\theta_x\cos\theta_z = 0, \tag{24}$$

and F_2 for

$$\frac{\partial F_2}{\partial\theta_x} = 0 \rightarrow \sin\theta_x + r\sin\theta_z\cos\theta_x = 0, \tag{25}$$

$$\frac{\partial F_2}{\partial\theta_z} = 0 \rightarrow r\gamma\sin\theta_z + \sin\theta_x\cos\theta_z = 0. \tag{26}$$

It is readily shown that condition (21) is always guaranteed since, for modes verifying (23),(24) (i.e., $(0,0)$, $(\pm\pi,\pm\pi)$, $(\mp\pi,\pm\pi)$, $(0,\pm\pi)$, $(\pm\pi,0)$), the inequality (21) is satisfied. As a result, the stability conditions will be obtained by imposing (22). By combining (25),(26), it can be shown that the extreme of F_2 is reached for modes $(0,0)$, $(\pm\pi,\pm\pi)$, $(\pm\pi,\mp\pi)$, $(0,\pm\pi)$, $(\pm\pi,0)$, and for modes verifying

$$\cos^2\theta_z = \gamma^2\frac{1+r^2}{1+\gamma^2r^2}, \qquad \sin^2\theta_z = \frac{1-\gamma^2}{1+\gamma^2r^2}, \tag{27}$$

$$\cos^2\theta_x = \frac{1+\gamma^2r^2}{1+r^2}, \qquad \sin^2\theta_x = \frac{\left(1-\gamma^2\right)r^2}{1+r^2}. \tag{28}$$

The most constraining condition for stability is given by modes (27),(28) which yield the minimal value

$$F_2 = 2 - 2d - 2\gamma\,dr^2 - 2d\sqrt{1 + (1+\gamma^2)\,r^2 + \gamma^2r^4}. \tag{29}$$

The stability condition is obtained as follows by imposing that F_2 is positive:

$$d\left(1 + \gamma r^2 + \sqrt{1 + (1+\gamma^2)\,r^2 + \gamma^2r^4}\right) \leq 1. \tag{30}$$

Two particular cases are of interest: the purely explicit scheme ($\mu = 0,\ \gamma = 1$) and the implicit vertical resolution ($\mu = 1,\ \gamma = -1$), the stability condition of which simplify to

$$\mu = 0 \rightarrow d\left(1 + r^2\right) \leq \frac{1}{2}, \tag{31}$$

$$\mu = 1 \rightarrow d \leq \frac{1}{2}. \tag{32}$$

With typical values of $\alpha = 10^{-2}$, $\kappa = 10^3\,\mathrm{m^2/s}$, $\Delta t = 10^5\,\mathrm{s}$, $\Delta z = 10\,\mathrm{m}$ (at surface), and $\Delta x = 10^5\,\mathrm{m}$ encountered in OGCMs corresponding to $r = 100$ and $d = 10^{-2}$, condition (31) is violated while (32) is trivially verified. As recommended by Cox [2], an implicit resolution of $D^{|}$ is therefore necessary for long-term climatic simulations. This, however, requires the resolution of a tridiagonal system at each time step.

In practice, in addition to computational stability, the numerical scheme is required to avoid oscillations in time. This property is obtained by imposing $G \geq 0$ (no flip-flop condition) rather than $G \geq -1$. By proceeding in a similar way as for the stability condition, we get the following no flip-flop condition where $\hat{\gamma} = 1 - \mu \in [0, 1]$,

$$d\left(1 + \hat{\gamma} r^2 + \sqrt{1 + (1 + \hat{\gamma}^2)\, r^2 + \hat{\gamma}^2 r^4}\right) \leq \frac{1}{2}. \tag{33}$$

For an implicit resolution of $D^{|}$, the stability condition simplifies to

$$d\left(1 + \sqrt{1 + r^2}\right) \leq \frac{1}{2}, \tag{34}$$

which, for large values of r, is asymptotic to

$$dr = \frac{\kappa \alpha \Delta t}{\Delta x \Delta z} \leq \frac{1}{2}. \tag{35}$$

The above no flip-flop condition is used to determine the limitation of the time step in our OGCM.

5. CONCLUSIONS

In this study, we have explored the numerical accuracy and stability of the Cox [2] scheme. Consistency of the scheme was shown to require an appropriate definition of the vertical grid. The scheme was shown to be first-order accurate in space on a nonuniform vertical grid. The truncation error in time is of first-order accuracy whatever the value of the implicitness factor μ. Properties of the spatial discretisation have been explored by studying the behaviour of Fourier modes in the numerical and continuous schemes. Finally, necessary stability and no flip-flop conditions were established for the time stepping used in CLIO. The need for an implicit resolution of the operator $D^{|}$ was underscored.

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