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Enforcing the Continuity Equation in Numerical Models of Geophysical Fluid Flows

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Abstract—A method is described for modifying the velocity field in geophysical fluid models so as to enforce the continuity equation. A corrective mass flux is introduced, which derives from a scalar potential. The latter is the solution of a Poisson problem which is formulated in such a way that a suitable norm of the corrective velocity be minimum. It is seen that a generalised vertical coordinate may be used. Finally, an elementary, one-dimensional illustration of the functioning of the method suggested is provided. © 2001 Elsevier Science Ltd. All rights reserved.

Keywords—Geophysical fluid flow, Continuity equation, Corrective velocity, Poisson problem.

1. INTRODUCTION

Numerical models of geophysical fluid flows often include routines for simulating the fate of dissolved constituents. Typically, the concentration of such a constituent obeys an advection/diffusion partial differential equation. A numerical algorithm for estimating the solution of an equation of this type is unlikely to be accurate if the density and velocity fields do not satisfy exactly the associated discrete version of the continuity equation—which is obtained by assuming that the concentration under study is equal to a constant at every time and location in the computational domain. In certain numerical models (e.g., [1]), the procedure for estimating the velocity field is such that this condition is not identically met. As a consequence, prior to computing the concentration of dissolved constituents, a corrective velocity must be introduced so as to enforce the continuity equation. This is explained in mathematical terms below.

Let \tilde{t} denote time; \tilde{x} and \tilde{y} represent horizontal Cartesian coordinates, while \tilde{z} is the vertical Cartesian coordinate. If ρ and $\tilde{\mathbf{u}}=(\tilde{u},\tilde{v},\tilde{w})$ denote the fluid density and the velocity—the components of which are given in the Cartesian reference frame—predicted by the equations of

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the model, the continuity equation reads

$$\frac{\partial \rho}{\partial \tilde{t}} + \frac{\partial (\rho \tilde{u})}{\partial \tilde{x}} + \frac{\partial (\rho \tilde{v})}{\partial \tilde{y}} + \frac{\partial (\rho \tilde{w})}{\partial \tilde{z}} + \tilde{e} = 0.$$
 (1)

The error \tilde{e} should be zero. If this is not the case, a correction to the velocity, $\tilde{\mathbf{u}}' = (\tilde{u}', \tilde{v}', \tilde{w}')$, must be evaluated a posteriori so that the modified velocity field, $\tilde{\mathbf{u}} + \tilde{\mathbf{u}}' = (\tilde{u} + \tilde{u}', \tilde{v} + \tilde{v}', \tilde{w} + \tilde{w}')$, satisfies

 $\frac{\partial \rho}{\partial \tilde{t}} + \frac{\partial \left[\rho \left(\tilde{u} + \tilde{u}'\right)\right]}{\partial \tilde{x}} + \frac{\partial \left[\rho \left(\tilde{v} + \tilde{v}'\right)\right]}{\partial \tilde{y}} + \frac{\partial \left[\rho \left(\tilde{w} + \tilde{w}'\right)\right]}{\partial \tilde{z}} = 0. \tag{2}$

Of course, it is $\tilde{\mathbf{u}} + \tilde{\mathbf{u}}'$ which must be used to compute the concentration of dissolved constituents. Combining equations (1) and (2) yields

$$\frac{\partial \left(\rho \tilde{u}'\right)}{\partial \tilde{x}} + \frac{\partial \left(\rho \tilde{v}'\right)}{\partial \tilde{y}} + \frac{\partial \left(\rho \tilde{w}'\right)}{\partial \tilde{z}} = \tilde{e}.$$
(3)

Herein a method is outlined for calculating the components of the corrective velocity which is based on the assumption that an appropriate norm of the corrective mass flux, $\tilde{\mathbf{u}}'$, should be as small as possible. Since a large fraction of geophysical fluid models resort to a non-Cartesian vertical coordinate, it is desirable to first reformulate the problem to be tackled in a coordinate system including a generalised vertical coordinate.

2. GENERALISED VERTICAL COORDINATE

A generalised vertical coordinate may be introduced as part of the following transformation of the independent variables (e.g., [2,3]):

$$(t, x, y, z) = \left[\tilde{t}, \tilde{x}, \tilde{y}, z\left(\tilde{t}, \tilde{x}, \tilde{y}, \tilde{z}\right)\right], \tag{4}$$

where the new variables are those devoid of tildes. Time and the horizontal coordinates are unaffected by the variable change above.

The first-order derivatives with respect to the independent variables transform to

$$\frac{\partial}{\partial \tilde{t}} = \frac{\partial}{\partial t} + \frac{\partial z}{\partial \tilde{t}} \frac{\partial}{\partial z},\tag{5}$$

$$\frac{\partial}{\partial \tilde{x}} = \frac{\partial}{\partial x} + \frac{\partial z}{\partial \tilde{x}} \frac{\partial}{\partial z},\tag{6}$$

$$\frac{\partial}{\partial \tilde{y}} = \frac{\partial}{\partial y} + \frac{\partial z}{\partial \tilde{y}} \frac{\partial}{\partial z},\tag{7}$$

$$\frac{\partial}{\partial \bar{z}} = \frac{1}{g} \frac{\partial}{\partial z},\tag{8}$$

where $g = (\frac{\partial z}{\partial \tilde{z}})^{-1}$ is the Jacobian of the coordinate transformation. Along with the new vertical coordinate, it is customary to introduce a new velocity field, defined to be

$$(u, v, w) = \left(\tilde{u}, \tilde{v}, \frac{\partial z}{\partial \tilde{t}} + \tilde{u} \frac{\partial z}{\partial \tilde{x}} + \tilde{v} \frac{\partial z}{\partial \tilde{y}} + \tilde{w} \frac{\partial z}{\partial \tilde{z}}\right). \tag{9}$$

Using relations (4)-(9), it may be seen that equations (1)-(3) read in the new independent variable system

$$\frac{\partial(g\rho)}{\partial t} + \frac{\partial(g\rho u)}{\partial x} + \frac{\partial(g\rho v)}{\partial y} + \frac{\partial(g\rho w)}{\partial z} + e = 0, \tag{10}$$

$$\frac{\partial(g\rho)}{\partial t} + \frac{\partial\left[g\rho\left(u+u'\right)\right]}{\partial x} + \frac{\partial\left[g\rho\left(v+v'\right)\right]}{\partial y} + \frac{\partial\left[g\rho\left(w+w'\right)\right]}{\partial z} = 0,\tag{11}$$

$$\frac{\partial (g\rho u')}{\partial x} + \frac{\partial (g\rho v')}{\partial y} + \frac{\partial (g\rho w')}{\partial z} = 0, \tag{12}$$

3. OPTIMIZATION PROBLEM

Clearly, the corrective velocity should be as small as possible. This is why it is suggested that it be evaluated in such a way that an appropriate norm of it be as small as possible. Let Ω and Γ represent the domain of interest and its boundary in the transformed space. As will be seen, the following norm is suitable:

$$V = \left(\frac{\int_{\Omega} \left[(g\rho u')^2 + (g\rho v')^2 + (g\rho w')^2 \right] d\Omega}{\int_{\Omega} (g\rho)^2 d\Omega} \right)^{1/2}, \tag{13}$$

where $d\Omega = dx\,dy\,dz$. For the integral above to be valid, it is necessary that w' have the dimension of a velocity, which requires that the transformed vertical coordinate z have the dimension of a length. In addition, for the contributions to the norm V of the vertical and horizontal motions to be of a similar order of magnitude, it is desirable that the typical height of Ω be of the same order of magnitude as its horizontal size. For instance, a vertical coordinate satisfying these conditions is easily obtained from the classical sigma-coordinate [4] by multiplying the latter by a constant scaling factor, the value of which is the order of magnitude of the typical horizontal size of the domain of interest.

As g and ρ are not affected by the procedure for correcting the velocity field, the minimum of V is obtained when the minimum of the integral

$$I = \int_{\Omega} |g\rho \mathbf{u}'|^2 d\Omega \tag{14}$$

is achieved, with $|g\rho \mathbf{u}'|^2 = (g\rho u')^2 + (g\rho v')^2 + (g\rho w')^2$.

It is convenient to impose that the transformed-space corrective mass flux $(g\rho u', g\rho v', g\rho w')$ derives from the scalar potential ϕ

$$(g\rho u', g\rho v', g\rho w') = \left(\frac{\partial \phi}{\partial x}, \frac{\partial \phi}{\partial y}, \frac{\partial \phi}{\partial z}\right). \tag{15}$$

Combining (12) and (14), the Poisson equation that must be satisfied by the potential ϕ at any point of Ω is obtained

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} = e. \tag{16}$$

To simplify notations, the transformed-space del operator $\nabla = (\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z})$ will be used wherever possible. Thus, for instance, (16) may be rewritten as

$$\nabla^2 \phi = e. \tag{17}$$

Moreover, substituting (15) into (14) and using the del operator, the integral to be minimized may be written as

$$I = \int_{\Omega} |\nabla \phi|^2 \ d\Omega. \tag{18}$$

It is appropriate to assume that the boundary Γ of the domain of interest consists of two parts, Γ^n and Γ^d . On the former, the normal velocity is imposed, so that the normal component of the corrective velocity must be zero. Hence, the boundary condition to be applied on Γ^n is a Neumann one which reads

$$\mathbf{n} \cdot \nabla \phi = 0,\tag{19}$$

where n is the unit outward normal vector to the boundary of the domain of interest. For instance, an impermeable surface belongs to the boundary fraction called Γ^n . On the other hand, on Γ^d ,

no constraint applies to the corrective velocity. As a result, this part of the boundary of the domain may be seen as "open". In other words, on Γ^d , the Dirichlet boundary condition

$$\phi = \Phi \tag{20}$$

may be prescribed while bearing in mind that function Φ is a priori unknown.

To summarize, the optimization problem to be solved is as follows: the function Φ is to be determined so that the potential ϕ satisfying Poisson equation (17) in Ω and boundary condition (19) on Γ^n minimizes integral (18).

4. SOLUTION

Without any loss of generality, ϕ may be split in two contributions

$$\phi = \gamma + \eta. \tag{21}$$

The function γ satisfies relations

$$\nabla^2 \gamma = e, \tag{22}$$

$$\mathbf{n} \cdot \nabla \gamma = 0, \tag{23}$$

and

$$\gamma = 0, \tag{24}$$

in Ω , on Γ^n , and on Γ^d , respectively. Then, taking (17) and (19) into account, it is readily seen that η must satisfy

$$\nabla^2 \eta = 0 \tag{25}$$

and

$$\mathbf{n} \cdot \nabla \eta = 0, \tag{26}$$

in Ω , and on Γ^n , respectively. Obviously, γ is defined unambiguously by relations (22)–(24), whereas η possesses degrees of freedom since its value on Γ^d , which is in fact Φ , is not prescribed a priori. Thus, the optimization problem to be solved may be reformulated as follows: given relations (21)–(24), Φ is to be determined in such a way that function η renders the integral (18) minimum while satisfying Laplace equation (25) in Ω and boundary condition (26) on Γ^n .

Substituting (21) into (18) yields

$$I = \int_{\Omega} \left(|\nabla \gamma|^2 + |\nabla \eta|^2 \right) d\Omega + 2J, \tag{27}$$

with

$$J = \int_{\Omega} \nabla \gamma \cdot \nabla \eta \, d\Omega. \tag{28}$$

Integrating by parts and using the divergence theorem, it is readily seen that J may be transformed to

$$J = \int_{\Omega} \left[\nabla \cdot (\gamma \nabla \eta) - \gamma \nabla^2 \eta \right] d\Omega$$
$$= \int_{\Gamma^n} \gamma \left(\mathbf{n} \cdot \nabla \eta \right) d\Gamma + \int_{\Gamma^d} \gamma \left(\mathbf{n} \cdot \nabla \eta \right) d\Gamma - \int_{\Omega} \gamma \nabla^2 \eta d\Omega. \tag{29}$$

By virtue of (26), (24), and (25), $\mathbf{n} \cdot \nabla \eta = 0$ on Γ^n , $\gamma = 0$ on Γ^d , and $\nabla^2 \eta = 0$ in Ω , respectively. Hence, the three contributions to integral J exhibited in (29) are zero, so that

$$J = 0. (30)$$

In other words, $\nabla \gamma$ is "orthogonal" to $\nabla \eta$ over the domain of interest Ω . Therefore, integral I simplifies to

 $I = \int_{\Omega} \left(\left| \nabla \gamma \right|^2 + \left| \nabla \eta \right|^2 \right) d\Omega, \tag{31}$

an expression which is minimum if and only if $\nabla \eta$ is zero at every location in Ω . Thus, function η must be equal to a constant, which is consistent with the relations (25),(26) that η must satisfy. Finally, the constant value of η may be assumed to be zero, since only the gradient of the scalar potential has an impact on the corrective velocity. As a consequence, for the minimum of integral I to be achieved, ϕ must be equal to γ , implying that function Φ must be zero. Hence, on Γ^d , the Dirichlet boundary condition to be enforced is

$$\phi = 0. \tag{32}$$

According to the developments above, the corrective velocity may be obtained by solving the following Poisson problem:

in
$$\Omega$$
: $\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial y^2} = e$,
on Γ^n : $\mathbf{n} \cdot \nabla \phi = 0$,
on Γ^d : $\phi = 0$,
 $(g\rho u', g\rho v', g\rho w') = \left(\frac{\partial \phi}{\partial x}, \frac{\partial \phi}{\partial y}, \frac{\partial \phi}{\partial z}\right)$.

5. ILLUSTRATION

An elementary illustration of the approach suggested in the present article is provided below. Assume that ρ and g are constant and that all variables are scaled to appropriate dimensionless forms. In a one-dimensional flow with constant density, the velocity must be constant. This is the only type of flow that guarantees that the error e is zero at any location of the computational domain. However, if the velocity is

$$u(x) = x, (33)$$

the error is

$$e = -1. (34)$$

Hence, a corrective velocity u'(x) is to be introduced. Obviously, the "divergence" of the latter must be

$$\frac{du'}{dx} = e = -1, (35)$$

implying that u'(x) is

$$u'(x) = U - x, (36)$$

where U is a constant.

Assume that the domain of interest is $0 \le x \le 1$, with open boundaries at x = 0 and x = 1. Then, the corrective velocity should be minimum in the sense that the integral

$$I = \int_0^1 (u')^2 \, dx \tag{37}$$

must be as small as possible. Substituting (36) into (37) yields

$$I = U^2 - U + \frac{1}{3}. (38)$$

The minimum of I over U is obtained for the value of U satisfying

$$\frac{dI}{dU} = 0. (39)$$

Hence, U = 1/2, so that

$$u'(x) = \frac{1}{2} - x. {(40)}$$

Therefore, the corrected, divergence-free velocity is

$$u(x) + u'(x) = \frac{1}{2}. (41)$$

The same result must be obtained by solving the differential problem for the potential ϕ , which is

$$\frac{d^2\phi}{dx^2} = -1,\tag{42}$$

$$\phi(x=0) = 0 = \phi(x=1), \tag{43}$$

the corrective velocity being related to ϕ by

$$u'(x) = \frac{d\phi}{dx}. (44)$$

It is readily seen that the solution of (42),(43) is

$$\phi(x) = -\frac{x^2}{2} + \frac{x}{2},\tag{45}$$

so that

$$\frac{d\phi}{dx} = \frac{1}{2} - x,\tag{46}$$

which is equivalent to (40), as expected.

An alternative version of this problem may be considered. If the boundary x = 0 is impermeable, the corrective velocity must be prescribed to be zero at this point. Thus, in (36), the constant U must be zero, leading to

$$u'(x) = -x \tag{47}$$

and

$$u(x) + u'(x) = 0. (48)$$

In this case, the boundary conditions on the potential ϕ are

$$\left[\frac{d\phi}{dx}\right]_{x=0} = 0\tag{49}$$

and

$$\phi(x=1) = 0. \tag{50}$$

The solution to equation (42) that satisfies the boundary conditions (49),(50) is

$$\phi(x) = -\frac{x^2}{2} + \frac{1}{2},\tag{51}$$

so that

$$\frac{d\phi}{dx} = -x,\tag{52}$$

which is consistent with (47).

6. CONCLUSION

The present method for enforcing the continuity equation through the introduction of a corrective mass flux enjoys the following properties.

- 1. The continuity equation applicable to a compressible fluid can be dealt with, as well as simplified forms of this equation, such as that used for an incompressible fluid—which simply requires that the divergence of the velocity is zero.
- 2. A generalised vertical coordinate can be used.
- 3. In most cases, it will be possible to set up a numerical scheme for solving the Poisson problem obeyed by the velocity potential that guarantees convergence toward a corrected velocity satisfying the continuity equation at an acceptable computational cost.

Although the calculations above are based on the philosophy that the corrective velocity should be as small as possible, only a global norm of this velocity was seen to be minimum. Thus, it cannot be excluded that in certain regions of the computational domain, the corrective velocity is found to be far from small. Whether or not such a problem would occur is most likely to depend on the particular problem to be solved, i.e., the form of the error e, the shape of the computational domain, and the nature of the boundary conditions. Therefore, it is probably impossible to assess the importance of this potential shortcoming by means of general developments, such as those included herein. This is why numerical tests should be conducted in the near future on models such as that described in [1].

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