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Numerical mass conservation in a free-surface sigma coordinate marine model with mode splitting

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ABSTRACT

When the mode splitting technique is used the variables playing a role in the mass conservation equation are computed with different frequencies, since two time steps are utilized. The three-dimensional velocity field advecting the scalar quantities must however be divergence free—in the time stepping of the scalar quantities. A simple method aiming at enforcing this condition is outlined in the case of a free-surface sigma coordinate model using a "forward time stepping". This technique consists in using the sum of the baroclinic transport at the old time step and the average of the barotropic transport over the baroclinic time increment. In the Appendix, one suggests another method, less accurate but capable of being used with any kind of time stepping.

Introduction

Most marine models involve the computation of scalar quantities, the governing equations of which are of the form

$$\frac{\partial a}{\partial t} + \nabla \cdot (\boldsymbol{u} a) + \frac{\partial (u_3 a)}{\partial x_3} = Q + D, \qquad (1)$$

where a, Q and D represent the scalar variable under study, an appropriate source/sink term and the diffusion term, respectively; $\mathbf{u}$ is the horizontal velocity vector and u_3 is the vertical component of the velocity; t and x_3 denote time and the vertical coordinate—pointing upwards—while ∇ is the horizontal "gradient operator", i.e., $\nabla = \mathbf{e}_1 \partial/\partial x_1 + \mathbf{e}_2 \partial/\partial x_2$, $\mathbf{e}_1$ and $\mathbf{e}_2$ being the horizontal unit vectors associated with the horizontal coordinates x_1 and x_2.

By elementary manipulations, Eq. (1), which is in "conservative form", may be cast into the so-called "advective form", i.e.,

$$\frac{\partial a}{\partial t} + \boldsymbol{u} \cdot \nabla a + u_3 \frac{\partial a}{\partial x_3} = Q_T + D, \qquad (2)$$

where the "total" production/destruction term is defined as

$$Q_T = Q - a\gamma, \qquad (3)$$

with

$$\gamma = \nabla \cdot \boldsymbol{u} + \frac{\partial u_3}{\partial x_3}. \qquad (4)$$

Of course, the continuity equation states that γ, the rate of divergence of the flow field, must be zero,

$$\gamma = 0, \qquad (5)$$

so that there is no need to introduce a correction to the source/sink term.

Nevertheless, as emphasized by many authors such as Patankar (1980, pp. 38, 39, 99), for instance, there are many numerical schemes in which Eq. (5) is not exactly satisfied, implying the presence of a spurious production/destruction term in evolution equations similar to Eq. (1).

In free-surface marine models using the sigma coordinate, the numerical counterpart of Eq. (5) is easily satisfied. However, when the mode splitting technique is utilized, providing the equations governing the evolution of scalar quantities with a divergence free flow field is not trivial. This objective may be achieved by resorting to an appropriate definition of the advection field, as is shown in the present note.

The sigma coordinate system

To take into account the topography of the bottom and the surface of the sea, it may be appropriate to use a coordinate system in which the lower and upper boundaries of the computational domain are coordinate surfaces. Building on the work of Kasahara (1974), Deleersnijder and Ruddick (1992) have presented a generalized vertical coordinate obeying this condition. A very popular particular case of this general coordinate system is the so-called "sigma coordinate" (Phillips, 1957; Freeman et al., 1972; Owen, 1980; James, 1986; Nihoul et al., 1986; Blumberg and Mellor, 1987; Deleersnijder, 1989; Davies, 1990; Beckers, 1991; Ruddick et al., 1993). The latter results from a linear coordinate transformation, which reads (Fig. 1)

$$\left(\tilde{t}, \tilde{x}_1, \tilde{x}_2, \tilde{x}_3\right) = \left(t, x_1, x_2, L\frac{x_3+h}{\eta+h} = L\sigma\right), \tag{6}$$

where the variables of the transformed space, or sigma space, are in the left-hand side of Eq. (6); h is the sea depth with respect to the reference sea level and η is the sea surface elevation so that $H = h + \eta$ represents the total height of the water column. The constant L is the sea depth in the sigma space and σ is a dimensionless vertical coordinate that is equal to 0 at the sea bottom and is equal to 1 at the sea surface.

Along with the sigma transformation, it is customary to introduce a new vertical velocity defined as

$$\tilde{u}_3 = \frac{\partial \tilde{x}_3}{\partial t} + \boldsymbol{u}\cdot\nabla\tilde{x}_3 + u_3\frac{\partial \tilde{x}_3}{\partial x_3}. \tag{7}$$

The impermeability of the sea surface and the sea bottom is easily expressed by

$$\left[\tilde{u}_3\right]_{\sigma=1,0} = 0. \tag{8}$$

It is convenient to adopt the following notations:

$$\left(\boldsymbol{U}, \bar{\boldsymbol{U}}, \hat{\boldsymbol{U}}, U_3\right) = \left(H\boldsymbol{u}, H\bar{\boldsymbol{u}}, H\boldsymbol{u} - H\bar{\boldsymbol{u}}, H\tilde{u}_3\right). \tag{9}$$

We call the variables above total transport, barotropic transport, baroclinic transport and vertical transport, respectively. In Eq. (9), $\bar{\boldsymbol{u}}$ denotes the depth-averaged horizontal velocity

$$\bar{\boldsymbol{u}} = \int_0^1 \boldsymbol{u}\,\mathrm{d}\sigma \tag{10}$$

In the sigma space, the continuity equation reads

$$H\gamma = \frac{\partial H}{\partial \tilde{t}} + \tilde{\nabla}\cdot\boldsymbol{U} + \frac{\partial U_3}{\partial \tilde{x}_3} = 0, \tag{11}$$

with $\tilde{\nabla} = \mathbf{e}_1\partial/\partial\tilde{x}_1 + \mathbf{e}_2\partial/\partial\tilde{x}_2$.

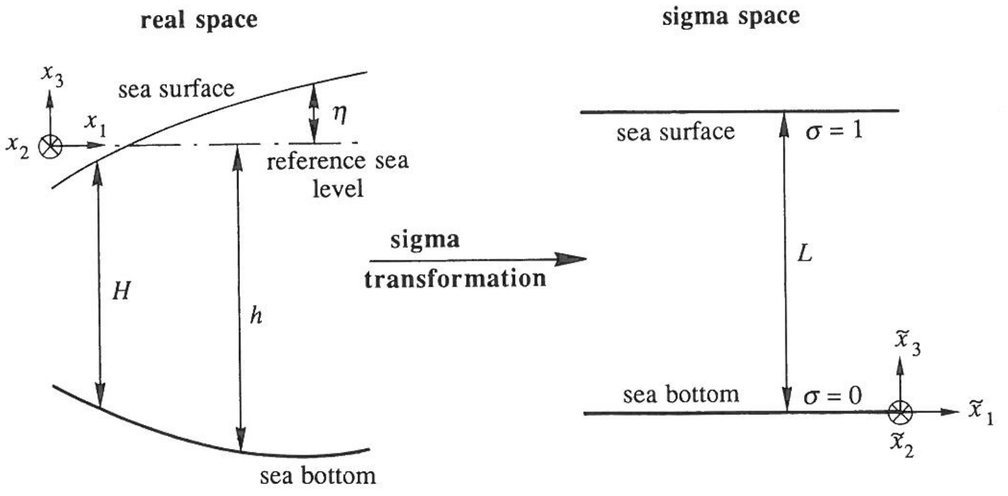

Fig. 1. Illustration of the sigma coordinate transformation.

Computation of scalar quantities

When using the sigma coordinate system, it is desirable to transform the typical evolution equation of scalar quantities (1) to

$$\frac{\partial Ha}{\partial \tilde{t}} + \tilde{\nabla} \cdot (\boldsymbol{U}a) + \frac{\partial (U_3 a)}{\partial \tilde{x}_3} = HQ + HD, \qquad (12)$$

This equation is in conservative form, which is usually preferable for robust numerical calculations and for preventing numerical loss or gain of the scalar quantity under study.

The flow field used in the left-hand side of Eq. (12) must satisfy the continuity Eq. (11), otherwise the spurious divergence or convergence of the flow field will give rise to artificial source / sink effects, as explained above. This condition must be satisfied by the numerical scheme, implying that the numerical discretization of the left-hand side of Eq. (12) must be such that

$$\begin{aligned} &\frac{\partial Ha}{\partial \tilde{t}} + \tilde{\nabla} \cdot (\boldsymbol{U}a) + \frac{\partial (U_3 a)}{\partial \tilde{x}_3} \\ &\quad = H\frac{\partial a}{\partial \tilde{t}} + \boldsymbol{U}.\tilde{\nabla} a + U_3 \frac{\partial a}{\partial \tilde{x}_3} + aH\gamma \\ &\quad = H\frac{\partial a}{\partial \tilde{t}} + \boldsymbol{U}.\tilde{\nabla} a + U_3 \frac{\partial a}{\partial \tilde{x}_3}. \qquad (13) \end{aligned}$$

Unfortunately, most numerical schemes, if not all of them, cannot verify Eq. (13), for the space discretization does not allow relations such as $\tilde{\nabla} \cdot (\boldsymbol{U}a) = \boldsymbol{U} \cdot \tilde{\nabla} a + a\tilde{\nabla} \cdot \boldsymbol{U}$ to hold valid. We are thus forced to turn to a less demanding test case. According to Patankar (1980, pp. 38, 39, 99), we will simply require that, when a is constant in space, the numerical scheme lead to

$$\frac{\partial Ha}{\partial \tilde{t}} + \tilde{\nabla} \cdot (\boldsymbol{U}a) + \frac{\partial (U_3 a)}{\partial \tilde{x}_3} = H\frac{\partial a}{\partial \tilde{t}}. \qquad (14)$$

We will thus require that the numerical schemes examined below successfully pass the test (14). The analysis will concentrate on the time discretization and it will simply be assumed that the space discretization is well-behaved, which means, for example, that $\tilde{\nabla} \cdot (\boldsymbol{U}a) = a\tilde{\nabla} \cdot \boldsymbol{U}$ holds true when a is constant in space.

From now on, all space derivatives are to be interpreted as their discretized counterparts.

The present study is mainly focused on time steppings involving "forward differences" in time.

Algorithm without mode splitting

We first examine a numerical scheme that does not resort to the mode splitting technique. In this case, it is not necessary to distinguish between $\bar{\boldsymbol{U}}$ and $\hat{\boldsymbol{U}}$—because these two parts of the total transport are computed with the same time stepping. Accordingly, the continuity Eq. (11) may be approximated by

$$\frac{H^{n+1} - H^n}{\Delta t} + \tilde{\nabla} \cdot \boldsymbol{U}^n + \frac{\partial U_3^n}{\partial \tilde{x}_3} = 0, \qquad (15)$$

where "n" refers to the instant $n\Delta$t, Δt being the time step.

An appropriate discretization of the left-hand side of Eq. (14) may be

$$\begin{aligned} &\frac{\partial Ha}{\partial \tilde{t}} + \tilde{\nabla} \cdot (\boldsymbol{U}a) + \frac{\partial (U_3 a)}{\partial \tilde{x}_3} \approx \frac{H^{n+1}a^{n+1} - H^n a^n}{\Delta t} \\ &\quad + \tilde{\nabla} \cdot (\boldsymbol{U}^n a^n) + \frac{\partial (U_3^n a^n)}{\partial \tilde{x}_3}. \qquad (16) \end{aligned}$$

Indeed, if a^n is constant, by virtue of Eq. (15), Eq. (16) may be transformed as follows:

$$\begin{aligned} &\frac{H^{n+1}a^{n+1} - H^n a^n}{\Delta t} + \tilde{\nabla} \cdot (\boldsymbol{U}^n a^n) + \frac{\partial (U_3^n a^n)}{\partial \tilde{x}_3} \\ &\quad = \left[\frac{H^{n+1}a^n - H^n a^n}{\Delta t} + \tilde{\nabla} \cdot (\boldsymbol{U}^n a^n) + \frac{\partial (U_3^n a^n)}{\partial \tilde{x}_3} \right] \\ &\qquad + H^{n+1}\frac{a^{n+1} - a^n}{\Delta t} \\ &\quad = a^n \left[\frac{H^{n+1} - H^n}{\Delta t} + \tilde{\nabla} \cdot \boldsymbol{U}^n + \frac{\partial U_3^n}{\partial \tilde{x}_3} \right] \\ &\qquad + H^{n+1}\frac{a^{n+1} - a^n}{\Delta t} \\ &\quad = a^n[0] + H^{n+1}\frac{a^{n+1} - a^n}{\Delta t} \\ &\quad = H^{n+1}\frac{a^{n+1} - a^n}{\Delta t} \approx H\frac{\partial a}{\partial \tilde{t}}. \qquad (17) \end{aligned}$$

Thus, the time stepping put forward above successfully passes the test (14).

Algorithm with mode splitting

When the mode splitting technique is used, two different time steppings coexist (Gadd, 1978; Madala, 1981; Blumberg and Mellor, 1987; Beckers, 1991). The barotropic mode—or external mode—, of which the variables are H and $\bar{U}$, is updated with the time step Δt_E, while the baroclinic mode—or internal mode—is concerned with the time step Δt_I. The numerical stability constraints being much more restrictive for the barotropic mode, we have

$$\frac{\Delta t_I}{\Delta t_E} = S, \tag{18}$$

where S is an integer number that is usually of order 10 to 100. We use the time index m for the baroclinic mode and the index n for the barotropic mode in such a way that (Fig. 2)

$$(m\Delta t_I, (m+1)\Delta t_I) = (n\Delta t_E, (n+S)\Delta t_E). \tag{19}$$

Because of the separation of the flow field variables into two categories concerned with different time steppings, it seems appropriate to split the continuity Eq. (11) into a barotropic and a baroclinic part. Integrating Eq. (11) over the water column, taking the impermeability conditions Eq. (8) into account, we obtain

$$\frac{\partial H}{\partial \tilde{t}} + \tilde{\nabla} \cdot \bar{U} = 0, \tag{20}$$

which involves the variables of the external mode only. Substracting Eq. (20) from Eq. (11) yields the "baroclinic continuity equation"

$$\tilde{\nabla} \cdot \hat{U} + \frac{\partial U_3}{\partial \tilde{x}_3} = 0. \tag{21}$$

Equation (20) permits updating the sea depth according to

$$\frac{H^{n+k+1} - H^{n+k}}{\delta t_e} + \tilde{\nabla} \cdot \bar{U}^{n+k} = 0,$$
$$k = 0, 1, \ldots, S-1. \tag{22}$$

It is suggested to discretize Eq. (21) as

$$\tilde{\nabla} \cdot \hat{U}^m + \frac{\partial U_3^m}{\partial \tilde{x}_3} = 0. \tag{23}$$

It is now essential to point out that the scalar quantities are updated with the time step of the baroclinic mode Δt_I. We thus have to provide the evolution equations of the scalar quantities with a flow field that verifies the discretized version of Eq. (11) in the baroclinic time stepping.

It would appear natural to use H^{m+1}, H^m, $\bar{U}^m$, $\hat{U}^m$ and U_3^m. But this set of variables does not verify the continuity Eq. (11). In the baroclinic time stepping, we indeed have

$$\frac{H^{m+1} - H^m}{\Delta t_I} + \tilde{\nabla} \cdot (\bar{U}^m + \hat{U}^m) + \frac{\partial U_3^m}{\partial \tilde{x}_3}$$
$$= \frac{H^{m+1} - H^m}{\Delta t_I} + \tilde{\nabla} \cdot \bar{U}^m = \frac{H^{m+1} - H^{n+1}}{\Delta t_I} \neq 0. \tag{24}$$

To obtain an appropriate set of variables, we first derive the following sum from Eq. (22):

$$\sum_{k=0}^{k=S-1} \left[\frac{H^{n+k+1} - H^{n+k}}{\Delta t_E} + \tilde{\nabla} \cdot \bar{U}^{n+k} \right] = 0, \tag{25}$$

which leads to

$$\frac{H^{m+1} - H^m}{\Delta t_E} + \tilde{\nabla} \cdot \left[\sum_{k=0}^{k=S-1} \bar{U}^{n+k} \right] = 0. \tag{26}$$

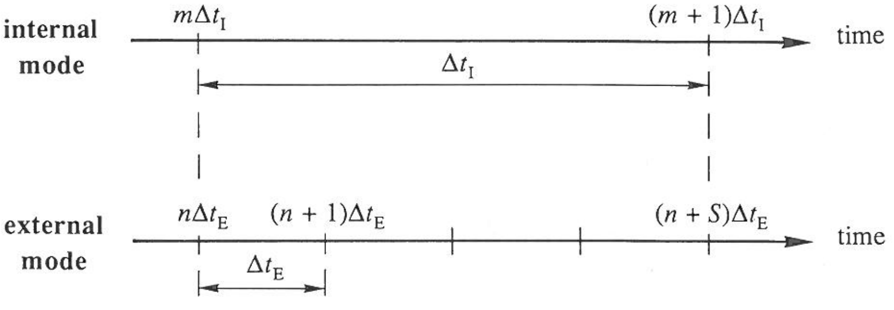

Fig. 2. Illustration of the baroclinic and the barotropic time steppings.

Then, we put

$$\mathbf{V}^m = \frac{1}{S} \sum_{k=0}^{k=S-1} \bar{U}^{n+k}, \tag{27}$$

which may be regarded as the average of the barotropic transport over one baroclinic time step. Dividing Eq. (26) by S, taking Eq. (27) into account, we have

$$\frac{H^{m+1} - H^m}{\Delta t_I} + \tilde{\nabla} \cdot \mathbf{V}^m = 0. \tag{28}$$

This enables us to define flow variables verifying the incompressibility condition. Indeed, adding Eqs. (23) and (28), we get

$$\frac{H^{m+1} - H^m}{\Delta t_I} + \tilde{\nabla} \cdot (\mathbf{V}^m + \tilde{U}^m) + \frac{\partial U_3^m}{\partial \tilde{x}_3} = 0. \tag{29}$$

The left-hand side of Eq. (14) may then be discretized as

$$\begin{aligned} &\frac{\partial Ha}{\partial \tilde{t}} + \tilde{\nabla} \cdot (Ua) + \frac{\partial (U_3 a)}{\partial \tilde{x}_3} \\ &\approx \frac{H^{m+1}a^{m+1} - H^m a^m}{\Delta t_I} + \tilde{\nabla} \cdot \left[(\mathbf{V}^m + \hat{U}^m) a^m \right] \\ &\quad + \frac{\partial (U_3^m a^m)}{\partial \tilde{x}_3}. \end{aligned} \tag{30}$$

Taking Eq. (29) into account, it is readily seen that, when a^{m} is constant, the discretization above transforms to

$$\begin{aligned} &\frac{H^{m+1}a^{m+1} - H^m a^m}{\Delta t_I} + \tilde{\nabla} \cdot \left[(\mathbf{V}^m + \hat{U}^m) a^m \right] \\ &+ \frac{\partial (U_3^m a^m)}{\partial \tilde{x}_3} = H^{m+1} \frac{a^{m+1} - a^m}{\Delta t_I} \approx H \frac{\partial a}{\partial \tilde{t}}. \end{aligned} \tag{31}$$

In other words, by defining the total horizontal transport as $\mathbf{V}^m + \hat{U}^m$, it is very easy to build a time stepping that successfully passes the test Eq. (14).

If the new baroclinic transport $\hat{U}^{m+1}$ is available when the scalar qantities are to be advanced in time, it might seem natural to use $\hat{U}^{m+1}$ instead of $\hat{U}^m$. To do so, it is sufficient to replace $(\hat{U}^m, U_3^{\mathrm{m}})$ by $(\hat{U}^{m+1}, U_3^{\mathrm{m}+1})$ from Eq. (21) on. It is easily understood that, with this slight modification, the method put forward here remains valid.

Conclusion

A method to deal with spurious flow convergence/divergence effects in the evolution equations of scalar quantities has been presented. As a matter of fact, it is guaranteed that these spurious effects will not arise only in regions where the scalar quantity under study exhibits negligible space variations. Since our method provides a divergence free velocity field in the time stepping of the internal mode, improvements in the numerical results are expected whatever the space distribution of the scalar quantities.

We have examined algorithms with and without mode splitting. In the latter case, one has to consider the sum of the baroclinic transport and the average of the barotropic transport over the baroclinic time step. The method proposed here is extremely simple and implies negligible extra computer costs.

The present discussion is focused on the computation of scalar quantities only. In other words, the problem of providing the momentum equations with a divergence free flow field has not been addressed. This is however not a major issue.

Our method is well suited to a “forward time stepping”. Nevertheless, it is unlikely to be of any use to other types of time steppings such as, for instance, the leapfrog technique. A general method is explained in the Appendix. It can be adapted to any kind of time stepping but it turns out to be less powerful than the method suggested above.

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Appendix

Here we suggest a method capable of providing the internal mode with a divergence free flow field whatever the type of the time stepping.

First, the scalar quantity Eq.(12) is solved by assuming that the right-hand member is zero and that a is constant in space and time. This leads to a value of the sea depth at the new time level, H_*^{m+1}, which is in general not equal to that obtained from the external mode equations, H^{m+1}. However, a divergence free flow field is now available in the time stepping of the internal mode. Then, with this flow field, the scalar quantity a is advanced in time, leading to the fictitious value a_*^{m+1}. Finally, the new value of a is derived from $a^{m+1}=(H_*^{m+1}/H^{m+1})a_*^{m+1}$, which allows correcting the sea depth value without changing the total amount of a contained in the computational domain.

This technique, yet fully general, has obvious shortcomings, which may be highlighted by considering an extremely simple case. It is hypothesized that Eq. (12) involves no source/sink term, i.e., $Q=0$. Further assuming that a is initially constant in space, it is readily seen that a must remain constant as time progresses. Unlike the method specifically designed for the forward time stepping, the general method cannot reproduce this behaviour, unless $H_*^{m+1}=H^{m+1}$ at any time and at any location, which would correspond to a truly exceptional—and probably useless—flow configuration.

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