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Stability constraints for oceanic numerical models: implications for the formulation of time and space discretizations

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ABSTRACT

Except for vertical diffusion (and possibly the external mode and bottom drag), oceanic models usually rely on explicit time-stepping algorithms subject to Courant–Friedrichs–Lewy (CFL) stability criteria. Implicit methods could be unconditionally stable, but an algebraic system must be solved at each time step and other considerations such as accuracy and efficiency are less straightforward to achieve. Depending on the target application, the process limiting the maximum allowed time-step is generally different. In this paper, we introduce offline diagnostics to predict stability limits associated with internal gravity waves, advection, diffusion, and rotation. This suite of diagnostics is applied to a set of global, regional and coastal numerical simulations with several horizontal/vertical resolutions and different numerical models. We show that, for resolutions finer that 1/2°, models with an Eulerian vertical coordinate are generally constrained by vertical advection in a few *hot spots* and that numerics must be extremely robust to changes in Courant number. Based on those results, we review the stability and accuracy of existing numerical kernels in vogue in primitive equations oceanic models with a focus on advective processes and the dynamics of internal waves. We emphasize the additional value of studying the numerical kernel of oceanic models in the light of coupled space–time approaches instead of studying the time schemes independently from spatial discretizations. From this study, we suggest some guidelines for the development of temporal schemes in future generation multi-purpose oceanic models.

1. Introduction

1.1. Context

Owing to advances in computational power, global climate models are now configured with increasingly higher horizontal/vertical resolution. The extension of the range of application of this type of model, originally developed for low-resolution large-scale configurations, raises some new challenges of numerical and physical nature (Griffies, 2013; Griffies and Treguier, 2013) and requires the accurate representation of a wider energy spectrum. Moreover, multi-resolution configurations via one-way or two-way nesting techniques are now mature (Debreu and Blayo, 2008; Debreu et al., 2012) and could be used to locally reach marginal submesoscales resolving resolutions (e.g. Marchesiello et al., 2011). Low-resolution configurations imply relatively slow and laminar (linear) flows while many emerging issues arise when extending the range to finer scales: the appropriate representation of internal wave dynamics is increasingly important to predict physical mixing (e.g. Arbic et al., 2012), the addition of biogeochemical tracers imposes new constraints on advection schemes (e.g. Lévy et al., 2001), adequate capture of the transfers between resolved and unresolved scales is required (Thuburn et al., 2014), spurious dianeutral mixing remains a key issue in the presence of mesoscale eddies (Ilicak et al., 2012). Another difficulty is the proper synergy between physical parameterizations and the numerics to ensure regularity of the physical solutions by limiting fine-scale variance (e.g. Hecht, 2010). More generally, high-resolution modeling requires a finer consideration of numerical methods. This has motivated the emergence of comprehensive initiatives like

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the COMODO[1] and DCMIP[2] projects aimed at intercomparison of numerical kernels to exploring the merits of different approaches through a suite of semi-idealized testcases.

The objective of this paper is to define the main guidelines for the development of temporal schemes in future generation multi-purpose (i.e. used for applications ranging from paleo-climate to eddying regimes) oceanic models. Because changing the time-stepping algorithm is one of the most fundamental change to an existing numerical code, it is legitimate to first proceed to a deep investigation of the requirements. Originally, for climate models, temporal discretizations were mainly chosen for their simplicity and upon additional criteria:

(i) Their ability to conserve quadratic quantities (e.g. energy, potential vorticity or enstrophy) when combined with specifically designed second-order centered schemes for non-linear momentum advective terms formulated in a vector invariant form of the shallow-water equations (e.g. Sadourny, 1975). This led to the choice of the Leapfrog scheme in the momentum equation to minimize dissipation. Energy and/or potential enstrophy conserving schemes are considered an efficient way to suppress nonlinear instabilities.
(ii) Conservation of the second moments (i.e. quadratic variance) for tracers which resulted in the use of centered-in-space and Leapfrog-in-time schemes for tracer advection.
(iii) For their computational efficiency (i.e. the stability range with respect to the number of computations of the rhs) for internal gravity waves. An efficient way for extending the stability range of Leapfrog based models is the pressure gradient averaging approach of Brown and Campana (1978) which is still being used in several numerical models (Griffies et al., 2000).

As a result, most numerical models were historically based on a leapfrog scheme for both the tracer and momentum equations, combined with second-order centered schemes. Note that, even if most models now favor the flux form to the vector-invariant form of momentum equations, it remains crucial to know as accurately as possible the discrete properties of numerical schemes in terms of energy dissipation to close the energy cycle (Eden et al., 2014).

When high-resolution turbulent regimes start emerging in numerical simulations the algorithmic choices must evolve beyond the Leapfrog-in-time—second-order in space framework to accommodate to new constraints (e.g. Shchepetkin and McWilliams, 2005). Indeed, as mentioned above, other important properties arise for finer resolution: accuracy, for correct shape preservation and phase speed, preservation of positivity hence good stability for advective and diffusive processes, good dissipation properties when high-frequency forcings are used, etc. This is especially true for terms integrated using explicit time-stepping but also for terms integrated using implicit methods (typically vertical/isoneutral diffusion and bottom drag) for which accuracy considerations should not be overlooked. In most existing numerical models, the space–time algorithms are derived by studying separately the space and time dimensions assuming the other dimension is continuous (i.e. the underlying partial differential equation is semi-discretized, e.g. Hundsdorfer and Trompert, 1994; Shchepetkin and McWilliams, 2005). There is, however, a second standard reasoning to derive space–time algorithms: the coupled space–time approach for which both space and time dimensions are discretized (e.g. Lax and Wendroff, 1960; Leonard, 1979; Daru and Tenaud, 2004). This approach is more tedious to use but is expected to provide a more accurate measure of the stability and numerical errors for a given sub-system of the full system of equations under consideration.[3] Indeed, this would serve little purpose to combine a low-order temporal scheme with a high-order space discretization. A clear advantage of the space–time approach is to combine errors associated with the space and time discretizations in the same study.

A long-standing belief is that a given process when integrated using small Courant numbers (compared to the CFL constraint) has inherently small numerical errors associated with the time-stepping algorithm. From this perspective, improving the order of accuracy of the time-stepping algorithm would not be a priority as long as sufficiently small time-steps are chosen. This statement is, however, inexact because it ignores the interaction between time and space discretization errors. It is not unusual to see space–time discretization schemes with large numerical errors for small Courant numbers and less errors close to their stability limit (e.g. a Leapfrog scheme combined with a second-order centered scheme). The objective of the present study is first to estimate the typical order of magnitude of Courant numbers encountered in realistic configurations. Then, using those estimates, we will proceed to a deep investigation of the behavior of space–time numerical schemes usually found in state-of-the-art oceanic models over a relevant range of Courant numbers. In this case, numerical schemes will be studied close to their functioning conditions found during realistic simulations.

A first step toward our objective is to determine which terms are expected to be the most important in terms of stability for a given target application. Using a scaling analysis, Griffies and Adcroft (2008) studied the time step constraints introduced by the Coriolis term, advection, internal gravity wave propagation, as well as biharmonic viscosity and harmonic diffusion with respect to the horizontal grid spacing. Their study suggests that the details of the numerical integration schemes must be considered to get a clear estimate of which process sets the time-step. For the typical resolution of today's climate models it is unlikely that inertial oscillations or the viscous/diffusive operators will be responsible for the time-step limitation. We, thus, focus our study on three-dimensional advection and internal gravity waves, assuming that the numerical models under consideration are discretized on a horizontal C-grid with an Eulerian vertical coordinate in the primitive equations limit. Moreover, we assume that sea-ice or external gravity waves (through the "leakage" of the barotropic mode (e.g. Griffies et al., 2000; Shchepetkin and McWilliams, 2005; Demange et al., 2014b)) do not contribute to the limitation of the maximum allowed time-step. Important notations used throughout the paper are summarized in Table 1.

1.2. Stability of numerical models

Throughout this paper, x and y are the horizontal directions aligned with the computational grid, z is the vertical coordinate oriented upward from the topography $-h_{i,j}$ to the free surface $\zeta_{i,j}$. We note $\mathbf{u} = (u, v, w)$ the three-dimensional velocity, w being the dia-surface velocity, and $\mathcal{V}$ the volume of a given grid cell

$$\mathcal{V}_{i,j,k} = \Delta x_{i,j,k} \Delta y_{i,j,k} \Delta z_{i,j,k}.$$

To formulate the stability constraint associated with three-dimensional advection, we need to define the volumetric fluxes $U_{i+\frac{1}{2},j,k}$, $V_{i,j+\frac{1}{2},k}$ and $W_{i,j,k+\frac{1}{2}}$, respectively in the two horizontal and vertical direction. Those fluxes are the velocities multiplied by the area of the corresponding grid cell face, i.e.

$$\begin{cases} U_{i+\frac{1}{2},j,k} = \Delta z_{i+\frac{1}{2},j,k} \Delta y_{i+\frac{1}{2},j} u_{i+\frac{1}{2},j,k} \\ V_{i,j+\frac{1}{2},k} = \Delta z_{i,j+\frac{1}{2},k} \Delta x_{i,j+\frac{1}{2}} v_{i,j+\frac{1}{2},k} \\ W_{i,j,k+\frac{1}{2}} = \Delta x_{i,j} \Delta y_{i,j} w_{i,j,k+\frac{1}{2}} \end{cases}$$

[1] French Numerical Ocean Modeling Community http://www.comodo-ocean.fr .

[2] Dynamical Core Model Intercomparison Project https://www.earthsystemcog.org/projects/dcmip/ .

[3] The coupled space–time approach is only viable when applied to selected terms in the equations; e.g. advection, gravity waves or Coriolis considered separately. It is not applicable to the primitive equations as a whole.