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Forward-in-time upwind-weighted methods in ocean modelling

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SUMMARY

The World Ocean presents a remarkably wide range of spatial and temporal scales within complicated domains. At larger scales, beyond a few tens of meters, the ocean circulation can be seen to separate into quasi-horizontal and vertical directions, with the magnitude of mixing differing by many orders of magnitude between the two. It is within this context, and with additional constraints of flux-conservation when used for coupled climate simulation, that transport schemes are placed within ocean general circulation models.

Forward-in-time upwind-weighted methods have made gradual, steady inroads into the field. We review this evolution from centred-in-time centred-in-space schemes, first discussing temporally hybrid models (centred discretization of the momentum equations with forward-in-time treatment of the scalar transport equations), then fully forward-in-time models, touching on a number of test problems and analyses that have provided guidance to these model development efforts and discussing selected results.

KEY WORDS: ocean modelling; general circulation modelling; finite difference methods; computational methods

1. INTRODUCTION

Computational simulation of the oceans with primitive equation models began with Bryan [1], who built on earlier work in atmospheric modelling, particularly that of Arakawa [2], establishing a line of models known as Bryan–Cox or Bryan–Cox–Semtner. There have been many

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advancements in model physics since Bryan's original work, with Gent–McWilliams mixing [3], the K-Profile Parameterization of vertical mixing [4] and anisotropic forms of horizontal viscosity figuring prominently. Improvements in grid discretization have been made as well [5, 6], yet the original centred leapfrog dynamical core is still there, at least as an option, in many of the models used today.

Centred schemes preserve variance, are formally non-dissipative, but they also suffer from dispersive error, with one consequence being a tendency to generate two-grid-point noise. Bryan *et al.* [7] explained that the grid-Reynolds and grid-Peclet numbers must remain less than or equal to 2 in order to ensure that dissipation is sufficient to control this grid-point noise (this argument can also be found in the book of Griffies [8, Chapter 18]). In practice this constraint is most often violated, and with reasonable justification: One generally does not want to heavily smooth the entire model solution in order to control unphysical oscillations at a relatively few problem points.

Problem points, however, remain problematic. Flux-corrected transport (FCT) for the tracer equations (referring to temperature, salinity and any passive tracers), based on the work of Zalesak [9], was brought into the GFDL Modular Ocean Model (MOM) by Gerdes *et al.* [10]. Zalesak's method of improving advective transport was built on centred leapfrog differencing, where the tracer field is transported from time $(n-1)$ to time $(n+1)$ with fluxes based on the tracer field at step (n), centred in time between the starting and ending times, but the corrective fluxes are donor cell in form, bring in a (first-order) upwind-biased weighting. The donor cell fluxes are evaluated from the lagged or $(n-1)$ time step, just as is done for stable implementation of the diffusive operator, making it a temporally hybrid model, with the momentum equations treated with a centred-in-time and centred-in-space discretization, but with the tracers equations taking a forward-in-time character.

The motivation given by Gerdes *et al.* for using FCT was the concern over unphysical extrema in the tracer fields, identified in the Gulf of Guinea. Similar concerns with spurious tracer extrema have since motivated its use in many modelling studies, and FCT remains a supported option in newer versions of the model code [6]. Concerns with unphysical extrema, oscillatory behaviour, temporal accuracy and data structure have motivated the development and subsequent use of other consistently forward-in-time upwind-weighted methods for tracer transport. A number of problems in ocean modelling have been addressed with fully forward-in-time dynamical cores, borrowed from the atmospheric modelling community, two of which are discussed below. There is also considerable activity now towards the development of fully forward-in-time dynamical cores for layered ocean models, where the requirement of maintaining positive-definite layer thickness leads one naturally to the method.

This paper is presented as a brief review of forward-in-time methods in ocean modelling, meant as a useful primer on the field, covering temporally hybrid models and development of fully forward-in-time dynamical cores. It was presented in abbreviated form within a conference session on geophysical application of the Multi-Dimensional Positive Definite Advection and Transport Algorithm (MPDATA [11]), and indeed MPDATA appears prominently in the realm of forward-in-time methods in ocean modelling, not only through the application of the advection scheme itself but also through related research into the stable and accurate incorporation of forcing terms [12] and efficient use of higher-order methods and flux limiting.

2. PRIMITIVE EQUATION OCEAN MODELS

The primitive equations are derived from the Navier Stokes equations, with hydrostatic and shallow approximations being made. The Boussinesq approximation is also usually, though not always, made. These issues are discussed thoroughly in Reference [8].

The horizontal model grid is generally fixed in time and space, and locally orthogonal, though sometimes with considerable flexibility in the placement of grid singularities so as to allow the global ocean to be discretized with well-controlled grid cell volumes (References [13, 14]; also, Reference [15, Figure 1]).

A defining characteristic of the oceans, relative to many other systems treated in computational fluid dynamics, is the degree to which mixing is suppressed in the vertical direction relative to the horizontal. This decomposition into directions of strong and weak mixing appears to be more precisely in the plane in which the locally defined potential density is constant, and the normal direction, which is generally close to, but not exactly, vertical [3].

In order to preserve the weak magnitude of vertical (or quasi-vertical) mixing, some seven or so orders of magnitude less than that in the isopycnal plane, one must ensure that implicit vertical dissipation associated with the numerical treatment of advection remains below physically acceptable values, an issue discussed by Hasumi and Suginohara [16] and later quantified by Griffies *et al.* [17], where the authors present a method for diagnosing the spurious mixing associated with vertical advection. Yamanaka *et al.* [18] examined the interplay between vertical advective error, convective instability and circulation. Oschlies [19] provided additional evidence for the importance of vertical advection, and in Reference [20] demonstrated that an apparent deficiency of ocean biogeochemical cycle models, termed 'equatorial nutrient trapping' by Najjar *et al.* [21], and which modellers interpreted as arising through an oversimplification of the biogeochemistry, was in fact largely the result of numerical error in vertical advection.

This defining oceanic characteristic of low mixing in the vertical direction lends great importance to the choice of vertical grid. Possible choices include: (1) The fixed vertical or z coordinate of the first primitive equation ocean model [1], still the most widely used vertical coordinate today; (2) transformed/stretched (the so-called sigma) coordinates, in which all available levels fill each column of ocean in a proportional manner; and (3) isopycnal coordinate ocean models in which the potential density of any one of the several layers is everywhere constant (in this case the vertical coordinate becomes Lagrangian, drifting up and down as a material surface). Hybrid vertical coordinate ocean models have also become important, where a fixed z coordinate is used in regions with strong vertical mixing, an isopycnal coordinate is used in regions with weak vertical mixing and the challenging problem arises of blending between the two very different coordinate systems [22].

An issue somewhat unique to ocean models is that of the wide disparity between the fastest wave speeds and the speed of the flow. Surface gravity (external) waves, while of minor influence on the circulation, travel at speeds of over 200 m/s, with velocity proportional to $\sqrt{gh}$, where g is the gravitational acceleration and h the depth of the ocean. This is fully two orders of magnitude faster than the most rapid oceanic jets.

Fortunately, the vertical structure of these fast external waves is simple enough to allow very nearly complete isolation through vertical averaging, with the fast mode contained within the vertically averaged set of 2-D equations. What is left from this modal decomposition as a remainder are 3-D equations that contain internal wave modes as their fastest component.

The 3-D 'baroclinic' momentum equations are generally solved explicitly, time step limited usually by the first baroclinic mode. The 2-D 'barotropic' equations are solved either using an explicit approach with many necessarily short time steps, or they are solved implicitly; in either case, however, the relatively tedious and costly approach need only be applied to a 2-D set of equations.

The primitive equations in spherical coordinates are of the form

$$\frac{\partial u}{\partial t} + \mathscr{L}(u) + \mathscr{M}_u - fv = -\frac{1}{\rho_0}\frac{\partial P}{\partial_x} + \mathscr{V}(u) \tag{1}$$

$$\frac{\partial v}{\partial t} + \mathscr{L}(v) + \mathscr{M}_v + fu = -\frac{1}{\rho_0}\frac{\partial P}{\partial_y} + \mathscr{V}(v) \tag{2}$$

where (u, v) represent the two horizontal components of momentum, $\mathscr{V}$ represents viscosity (strongly anisotropic, as discussed above), f is twice the projection of the earth's rotation vector onto the local vertical at latitude ϕ,

$$f = 2\Omega \sin(\phi) \tag{3}$$

the $\mathscr{M}$'s are metric terms associated with the spherical geometry (see, for instance, References [5, 23]), P is the hydrostatic pressure,

$$P = \int_0^z \rho g \, \mathrm{d}z \tag{4}$$

integrated from the surface to depth z. The density ρ which appears in Equation (4) is a nonlinear function of temperature, salinity and depth (see, for example, Reference [24, Appendix Three]); if the Boussinesq approximation is made then a typical density ρ_0 is used elsewhere, where not multiplied by the g of gravity. Finally, the advection operator is

$$\mathscr{L}(u) = \nabla \cdot (\mathbf{u}u) \tag{5}$$

where the continuity equation has been used with the assumption of incompressibility,

$$(\nabla \cdot \mathbf{u}) = 0 \tag{6}$$

in order to commute $\mathbf{u}$ with the divergence operator.

Through the years, different techniques have been found for dealing with this separation into fast barotropic and slow baroclinic modes ([1, 25–27]; Higdon and de Szoeke [28] discuss the consequences of the inexactness of the decomposition and offers a prescription for stabilizing the approach), but one way or another it always is done in three-dimensional production-class ocean models. For example, following the approach taken in the Parallel Ocean Program (POP [5]), such a splitting could be implemented with the following set of substeps comprising one time step. With horizontal indices suppressed but a vertical index k indicated as needed:

1. First, the momentum equations are solved, but without the surface pressure gradient, to produce an auxiliary velocity $\mathbf{u}'(k)$.

2. Next, the vertical average of this auxiliary velocity is subtracted off, producing the 'baroclinic velocity' $\tilde{\mathbf{u}}'(k)$:

$$\tilde{\mathbf{u}}'(k) = \mathbf{u}'(k) - \bar{\mathbf{u}}' \tag{7}$$

   where the overbar implies a vertical average.
3. The vertically averaged equations of motion are solved for

$$\mathbf{U} = \bar{u} \tag{8}$$

   This substep is accomplished either with a number of small explicit time steps, subcycling over the longer baroclinic time step, or else with an implicit step.
4. Finally, the vertical average of the velocity (containing the fast external gravity waves associated with the surface pressure gradient) and the three-dimensional departure from that vertical average are recombined, as

$$\mathbf{u}(k) = \tilde{\mathbf{u}}'(k) + \mathbf{U} \tag{9}$$

The effectiveness of the modal decomposition rests in the isolation of the fast surface gravity waves to the two-dimensional set of equations which are solved in step (3). In various explicit or semi-explicit ocean models the details of the decomposition may differ, but some sort of vertical averaging will be done in order to treat the fast mode in isolation.

3. UPWIND-WEIGHTED FORWARD-IN-TIME TRACER ADVECTION

Ocean modellers consider tracers to include any passive scalar transported by the flow (chlorofluorocarbons or nutrients, for example), but also refer to potential temperature and salinity (or even density, in models that explicitly transport density) as tracers, even though they play a role in the dynamics through the pressure gradient terms appearing in Equations (1) and (2).

The equation for any transported tracer ψ is similar to the momentum equations, Equations (1) and (2), yet simpler:

$$\frac{\partial \psi}{\partial t} + \mathscr{L}(\psi) = \mathscr{D}(\psi) + \mathscr{S}(\psi) \tag{10}$$

where $\mathscr{D}$ represents diffusive terms (again, strongly anisotropic), $\mathscr{S}$ represents any source or sink terms, and

$$\mathscr{L}(\psi) = \nabla \cdot (\mathbf{u}\psi) \tag{11}$$

Soon after the introduction of FCT for tracer transport in ocean models [10, 29] the advantages of upwind-weighting of tracer advection in Equation (11) were explored further by Farrow and Stevens [30]. They motivated the need for improved tracer advection through examination of the confluence of the Brazil and Malvinas currents, identifying spurious extrema that were greatly reduced when the centred-in-time-and-space tracer advection was replaced with their upwind-weighted scheme. Their implementation was forward-in-time or two time-level, in the sense of requiring only one time-level of the tracer field to solve Equation (10), but followed a predictor-corrector sequence of two passes.

In the same year a wider consideration of advection schemes for application to ocean modelling was presented in the test problem of Hecht *et al.* [31]. The particular time-independent flow they used was that of an idealized single gyre with western boundary intensification described in an analytical form by Stommel [32], in a seminal paper in which he considered a simple analytical wind forcing balanced by linear bottom drag and showed that western boundary jets result from the meridional variation of the Coriolis parameter, or beta effect. Stommel's gyre solution, with its intensely sheared boundary current and relatively gentle interior flow, shares some of the qualities of the highly sheared counter rotating test problem of Smolarkiewicz [33], but in a context more clearly oceanic in nature.

Soon after the 1995 work of Hecht *et al.* [31], the so-called third-order upwind-weighted schemes came into wide-spread use in the tracer equations, based on the influential paper of Leonard [34]. These schemes use three-point interpolants, with the interpolation done either at the cell face, in the scheme Leonard referred to as QUICK, or at a point mid-way between the cell face and the estimated departure point. They are spatially second-order accurate except in the purely academic case of spatially uniform flow, in which case the fluxes are truly third-order accurate, yet the 'third-order' name remains widely used. The author has verified second-order convergence [31], but is unaware of any demonstration of third-order convergence, even for the problem of uniform flow and a smooth initial condition (see Reference [12] for commentary on the inability of third-order accurate fluxes to produce third-order convergence in one such test).

The leading error in these third-order upwind schemes is dissipative, in contrast to the dispersive error of centred schemes. This change in the fundamental character of the schemes, brought on only by adding a third point to the interpolation of tracers at the cell face, but with that third point taken from the upwind direction, can be readily understood if one decomposes the QUICK scheme into a centred-in-space term and a residual. If the centred-in-space term is taken to be fourth-order then the remainder is found to be a biharmonic (square of Laplacian) dissipative term with a velocity-dependent coefficient. At this point one can see the stability-based argument for a mixed temporal implementation of QUICK, with the centred-in-space portion applied centred-in-time, and the biharmonic remainder applied forward-in-time.

This spatial decomposition and mixed temporal application was presented by Holland *et al.* [35], but they noticed no particular advantage over a simpler uniformly centred-in-time implementation, an issue brought back into question in the 2000 paper of Hecht *et al.* [36]. A similar decomposition was discussed and adopted by Webb *et al.* [37], and remains in use in the OCCAM model (http://www.soc.soton.ac.uk/JRD/OCCAM/).

The third-order QUICK interpolant can alternatively be decomposed into a second-order centred-in-space term and a remainder which involves partial derivatives not of second-order, as in a Laplacian form, nor of fourth-order, as discussed above, but instead is in the less-familiar form of a third-order dissipative term with a velocity-dependent coefficient. This decomposition was adopted in the Modular Ocean Model [38], with the second-order-centred term applied centred-in-time and the remainder implemented forward-in-time. Referred to as QUICKER, this version of third-order upwind-weighted advection has remained an option in MOM [6].

The other third-order upwind scheme described in the 1979 paper of Leonard [34], known as QUICKEST, is more intrinsically oriented towards fully forward-in-time application, with the three-point interpolation being done between the cell face and the estimated departure point, at what would be the mid-point of that trajectory. In 1998, Hecht *et al.* [39] applied the one-dimensional QUICKEST scheme within a three-dimensional primitive equation model using time-splitting with error correction, following the explicitly error-corrected approach of Hunsdorfer and Trompert [40] in which second-order spatial accuracy is recovered for multi-dimensional use through systematic cancelation of leading-order errors identified through a Taylor series expansion.

The passive tracer test problem of Hecht *et al*. [31] was modified in Reference [36], rotating Stommel's gyre 45° relative to the grid, such that the fast western boundary current was skewed relative to the principal grid axes, producing a more effective multi-dimensional test. This modified test problem, some results of which are reproduced here in Figure 1, with brief discussion of the results in the figure caption, produced two new findings: (1) The centred-in-time application of QUICK described in Reference [35] and used within the ocean of the Community Climate System Model proved to be unstable, and (2) the time-splitting of one-dimensional schemes with correction of just the leading-order errors was shown to be undesirable, as the error-correction technique is ineffective in the under-resolved western boundary current region (as seen in Figure 1(d)).

At this point there were essentially three choices for tracer advection in primitive equation ocean models: centred-differencing, FCT and non-flux-corrected third-order upwind schemes. Strict monotonicity, while not always essential for the transport of density or its constituents, is a desirable quality, or may even be a requirement, for biogeochemical ocean modelling and other applications involving passive tracers (in some applications just sign-preservation may be sufficient, in which case the basic form of MPDATA is attractive).

In flux-limiting the lower-order flux is generally first-order donor cell upwind. The higher-order flux in FCT is the usual centred flux, yet there are advantages to having an upwind-weighting of the high-order flux as well. In FCT, the flux limiter is very active, with the resulting solution looking very different than it would without limiting. When an upwind-weighted scheme is flux-limited the limiter is much less active and the solutions produced with and without limiting are much more similar, making the impact on the solution of limiting more readily understood. The issues associated with consistency of phase space errors, with flux-correction of higher-order centred or upwind-weighted fluxes, are discussed in Section 4 of Reference [41].

Flux-limiting algorithms are expensive. One way of greatly reducing the overall cost of tracer advection was explored in Reference [39], with the idea of supercycling, or use of longer time steps for passive tracers than for active tracers. Even though the fastest mode may have been removed from the 3-D momentum equations through the modal decomposition mentioned in Section 2, the time step in the tracer equations may still be limited more strongly by the speed of the first internal wave mode rather than it would be by the Courrant–Friedrichs–Lewy condition (CFL [42]). In cases where CFL allows a time step two or more times longer than that allowed by the first internal mode supercycling presents an obvious cost-savings for any passive tracers, using either instantaneous or time-averaged advecting velocities. This was demonstrated with MPDATA, using the flux-limiting presented by Smolarkiewicz and Grabowski [41].

Supercycling has seen limited use, due to the existence of a competing technique which also accelerates the evolution of the dynamical tracers. This technique, which goes back to Bryan *et al*. [7], and has been analysed for ocean climate modelling application by Danabasoglu *et al*. [43] and Danabasoglu [44], can be thought of, in the case of the advection of temperature, as an artificial reduction in heat capacity (or salt capacity, in the case of salt

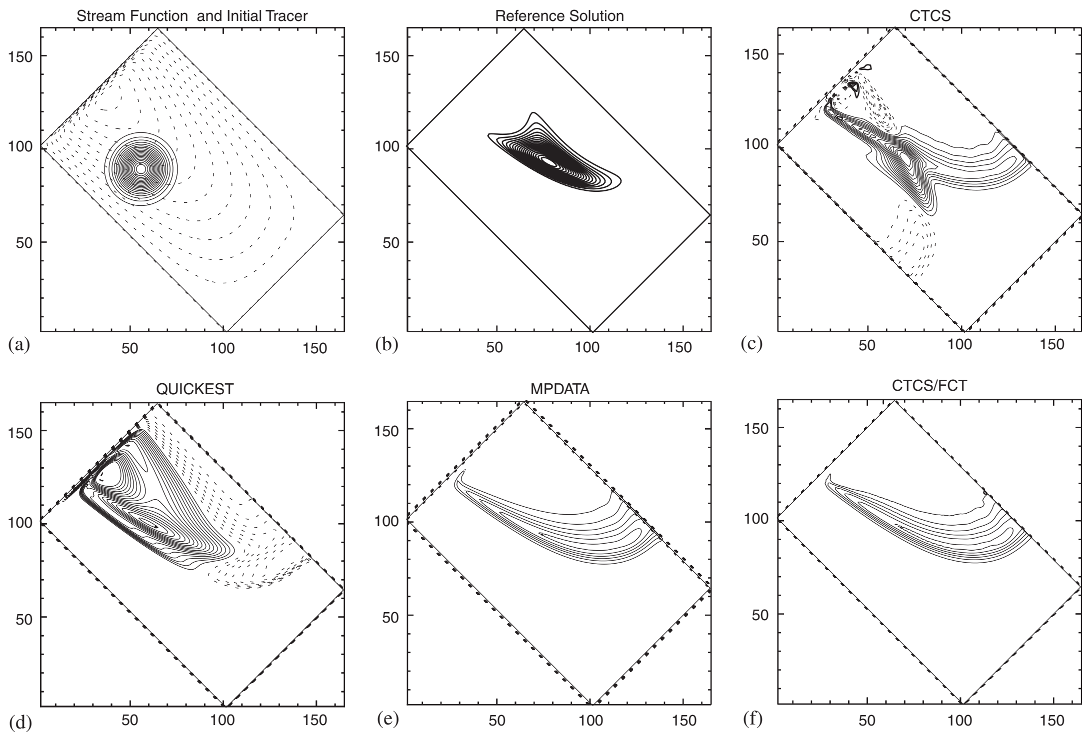

Figure 1. (a) Stream function (dashed) for the Stommel Gyre test problem, with initial Gaussian tracer distribution (solid contours). Orientation of flow is clockwise. Contour intervals are uniform for both stream function and tracer concentration (units are unimportant here). (b) Reference solution, produced following the method of characteristics. The reference solution can be considered to be exact, relative to the inexactness associated with the numerical advective error of solutions (c)–(f), produced with various advection schemes, as indicated. In these four panels tracer concentrations falling below that of the initial condition are shown with dashed contours. The centred-in-time centred-in-space scheme (panel (c)), still used in many ocean models, suffers from dispersive error, as is well-known. The dimensionally split QUICKEST scheme also produces extensive regions of tracer concentration below that of the initial condition, and qualitatively has produced three local maxima when there should be only one, as seen in panel (d). In contrast, the MPDATA and Flux Corrected Transport schemes shown in panels (e) and (f) are understood as producing qualitatively correct solutions, with slight dissipative error from the tracer distribution's pass through the intense western boundary current region dispersing the tracer concentration as it reaches regions of slower flow, where stream lines spread, as seen here. Reprinted from Reference [36], Copyright 2000, with permission from Elsevier.

transport), and is implemented simply through the use of two different time steps in an otherwise unchanged ocean model, with the artificially longer step appearing in the tracer equations. It is referred to as acceleration of tracers relative to momentum, though it should perhaps more accurately be thought of as deceleration of momentum relative to tracers, and it owes its success to the primary role of geostrophic balance in the oceans (the momentum equations adjust rapidly to the imposed pressure gradient).

There may yet be a place for the use of supercycling in tracer-rich biogeochemical modelling, as it avoids distortion of the dynamics and preserves an unambiguous definition of time, useful, for instance, in hindcasting and forecasting. The technique continues to see use in at least one such application (Bleck, private communication).

One additional issue concerning the temporal implementation of tracer advection in ocean climate models is that a number of the fluxes passed between the ocean and the other physical models (primarily but not limited to the atmospheric model), when integrated over the spatial domain and over time, must be strictly conserved between models.

4. SPECIAL PROJECTS IN OCEAN MODELLING

We move on now to discuss models in which the complete dynamical core is cast in a two time-level structure, entirely forward-in-time. In Section 5, this will bring us to isopycnal models and hybrid vertical coordinate models, after we discuss here two special projects in ocean modelling utilizing fully upwind-weighted forward-in-time atmospheric models, both built around MPDATA and applied to problems of oceanographic interest.

The first of these special projects, designed as an efficient and accurate method of integration and shown to be useful for some problems containing multiple timescales, was motivated by the idea of supercycling, described towards the end of the last section. The method of averages [45], or MOA, the concept was motivated as follows: In fluid problems where wave speeds are faster than the flow and yet the fastest waves are not of much importance overall to the dynamics, one could transport not only passive tracers through a long time step using a time-averaged velocity, as was demonstrated in the investigation of supercycling, above, but all the prognostic variables could be transported through long time steps restricted only by the CFL limit if the transporting velocity were low-pass filtered, exerting control over the problematic fastest waves. For example, the method could be applied to the primitive equations (our Equations (1) and (2)), as an illustrative if less efficient alternative to the barotropic/baroclinic mode splitting described in the steps surrounding Equations (7)–(9).

The problem is that the advecting velocity, even in what we call two-time-level schemes, should be at the mid-point of the interval between times n and $(n + 1)$. This mid-point velocity is often estimated through extrapolation Reference [46] and references therein). In MOA, two passes are made through the solution, first using a low-order scheme resolving the fast waves, then again with a high-order scheme through a single long time step, but with a low-pass filtered advecting velocity produced from the first low-order integration. Donor cell differencing was used as the inexpensive, low-order scheme in the first pass, enabling a high accuracy MPDATA scheme to be used in the second pass with a long time step, approaching the advective CFL limit. The authors demonstrated the method on a problem involving Rossby wave propagation and subsequent impact against the edge of a closed basin, setting off Kelvin waves which then circle the boundary, reproducing the results of Milliff and McWilliams [47], but using MOA.

The fact that the accuracy of integration of stiff systems is effectively addressed by MOA has come to be appreciated; see References [48, 49]. The method has also been used in a forest fire modelling code [50].

A descendant of the atmospheric modelling code used in the MOA study, recast as a flexible research code named EULAG [51, 52] in which the user can choose either Eulerian or semi-Lagrangian integration, has been applied to a number of focused problems. The model was used in non-hydrostatic mode to study the breaking of internal solitons generated by tides in the Mediterranean's Gulf of Gioia [53]. The model has also been used to numerically simulate the rotating tank experiments of Baines and Hughes [54] in order to better understand the process of western boundary separation; this work is discussed in brief in Reference [55].

5. ISOPYCNAL AND HYBRID COORDINATE MODELS

Isopycnal ocean modelling, in which the vertical coordinate is the potential density, and transport of potential temperature and salinity is constrained so as to maintain constant density within individual layers which are stacked one on top of the other, is particularly effective at maintaining water mass properties where diabatic mixing is very weak, as is the case over most of the volume of the oceans. The field was pioneered by Bleck and Smith [25], with the introduction of the Miami Isopycnal Ocean Model (MICOM, http://oceanmodeling.rsmas.miami.edu/micom/). This new direction for ocean modelling was an outgrowth of Bleck's earlier work in isentropic atmospheric modelling [56], which also led into the Rapid Update Cycle operational weather prediction model [57].

Many z coordinate ocean models have upwind-weighted forward-in-time advection of tracers as an option, as discussed above. Ocean models with an isopycnal character, in contrast, all have dynamical cores which are to some extent built around upwind-weighted transport, due to their need for flux limiting to prevent the thickness of thin layers from becoming negative.

Flux-corrected transport has been used in MICOM for mass transport, bringing in upwind-weighting, with the donor cell-based flux-limiting preventing the negative layer thicknesses even within the three-time-level leapfrog temporal framework. The model has been temporally hybrid, with advection of tracers being fully forward-in-time, since the work of Drange and Bleck [58] in which they described a variant of MPDATA.

Three other layered ocean models, documented in the literature but perhaps still considered to be research-class, as opposed to production class, have fully forward-in-time upwind-weighted dynamical cores and will be influential in determining the form of ocean models in coming years.

The Hallberg Isopycnal Model (HIM, http://www.gfdl.noaa.gov/rwh/HIM/HIM.html), which has been used now within some significant oceanographic studies [59], is based on the robust method of operator splitting of one-dimensional transport schemes for multi-dimensional use of Easter [60].

The Parallel Oregon State University Model (POSUM, http://posum.oce.orst.edu/), in which alternatives to potential density for layered ocean modelling have been explored [61], uses a forward scheme for tracers with a forward–backward method for mass transport.

The third of these models was presented by Higdon [62]. MPDATA was used throughout, and the robustness of the predictor-corrector approach to updating variables was demonstrated in a simple channel flow test problem in which a centred leapfrog dynamical core entirely fails, apparently due to difficulty with thin layers without engineering fixes to stabilize the model.

Experience with isopycnal ocean models has steadily grown, both in ocean-only (e.g. References [63–66]) and in coupled climate applications (see the simulated North Atlantic thermohaline circulation under increasing CO_2 of Figure 9.21 in Reference [67], with the most resilient circulation coming from the one climate model with an isopycnal ocean [68]; also see References [69, 70] for more recent, ongoing coupled climate simulations), and these results demonstrate certain advantages relative to the still more widely used z coordinate models. In an effort to capture the best of both z coordinate and isopycnal layer models, Bleck [22] has blended the vertical coordinate between z and isopycnal, an idea that was reclaimed from early work in wind-forced ocean modelling [71], which in turn represented Bleck's independent discovery and extension of an approach to blending flow-following Lagrangian and fixed Eulerian grids known elsewhere in computation fluid dynamics as the Arbitrary Lagrangian Eulerian technique (ALE [72]). The resulting HYbrid Coordinate Ocean Model (HYCOM, http://hycom.rsmas.miami.edu/) adopts most of the dynamical core of MICOM.

Recently, both MICOM and HYCOM have been used with FCT applied to potential temperature transport as well as to mass, based on Iskandarani's finding that it is preferable to use the same transport scheme consistently (Bleck, private communication). On the other hand, Higdon's model, developed as an alternative, fully two-time-level dynamical core for MICOM and HYCOM, has seen further refinement [73]. Results confirming its stability, even when used with no explicit dissipation, are reproduced here in Figure 2.

A second development effort on hybridized z and isopycnal coordinates, using an ALE approach, is being pursued at Los Alamos National Laboratory (http://climate.lanl.gov), where the HYbrid coordinate Parallel Ocean Program (HYPOP) has a two-time-level dynamical core with a predictor-corrector implementation which is similar to that of the Higdon's, with a modal decomposition [74] which is slightly different from that of HYCOM [25]. In both of these hybrid coordinate ocean models, the algorithms for determining the vertical grids, with the particular blending of Lagrangian isopycnal and Eulerian z grids, and for mapping the solution from old to new grids, are of essential importance, and are likely to see refinement in the coming years. The process of mapping between grids is one that readers may find

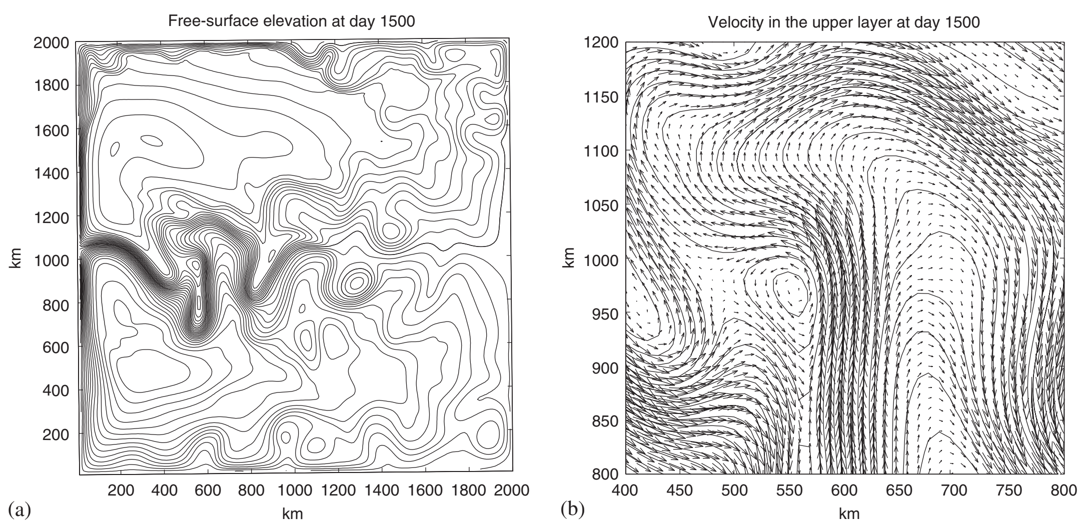

Figure 2. Results from a two-layer double-gyre wind-forced simulation with no explicit viscosity, from Reference [73]: (a) free surface elevation; and (b) a close-up view of upper layer velocity vectors with contours of the same free surface elevation. Reprinted from Reference [73], Copyright 2005, with permission from Elsevier.

interesting, even if it goes beyond the range of this paper: This mapping has much in common with advection, as discussed by Margolin and Shashkov [75] and the references therein.

6. CONCLUSIONS

The most important distinguishing feature of a primitive equation ocean model is its vertical grid. The most widely used vertical coordinate remains a fixed cartesian, or z grid. Upwind-weighted methods are in common use for scalar transport in such models, at least as an alternative to what may be the default centred leapfrog method. The treatment of the momentum equations in z coordinate models generally remains centred leapfrog.

In layered ocean models, on the other hand, the use of flux-limited transport schemes is not so much optional as fundamentally necessary, due to the requirement of maintaining positive definite layer thicknesses and conserving tracer in a variable-thickness environment. All layered ocean models have some sort of upwind-weighting of transport, and so it has not been such a great leap to fully forward-in-time dynamical cores.

Unquestionably there are opportunities, for researchers from within ocean modelling and from other areas of computational fluid dynamics, to contribute to the dynamical core of layered and hybrid layered-z-coordinate ocean models, so long as the issues unique to ocean modelling, such as the barotropic/baroclinic mode splitting, the disparity between the magnitudes of quasi-horizontal and vertical mixing and the importance of the choice of vertical coordinate, are understood. It is hoped that this paper presents a useful, if short, primer for those who may endeavour to improve dynamical cores for ocean modelling.

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REFERENCES

1. Bryan K. A numerical method for the study of the circulation of the World Ocean. *Journal of Computational Physics* 1969; **4**:347–376.
2. Arakawa A. Computational design for long-term numerical integration of the equations of fluid motion: two-dimensional incompressible flow. Part I. *Methods in Computational Physics* 1977; **17**:174–265.
3. Gent PR, Willebrand J, McDougall TJ, McWilliams JC. Parameterizing eddy-induced tracer transports in ocean circulation models. *Journal of Physical Oceanography* 1995; **25**:463–474.
4. Large WG, McWilliams JC, Doney SC. Oceanic vertical mixing: a review and a model with a nonlocal boundary layer parameterization. *Reviews of Geophysics* 1994; **32**:363–403.
5. Smith RD, Gent P. Reference manual of the parallel ocean program (POP). *Los Alamos National Laboratory Report LAUR-02-2484*, Los Alamos National Laboratory: Los Alamos, NM, 2002. Ocean Component of the Community Climate System Model (CCSM2.0).
6. Griffies SM, Harrison MJ, Pacanowski RC, Hallberg RW. A technical guide to MOM4. *GFEL Ocean Group Technical Report 5*, NOAA/Geophysical Fluid Dynamics Laboratory, 2004. Available on-line at http://www.gfdl.noaa.gov/fms.
7. Bryan K, Manabe S, Pacanowski RC. A global ocean-atmosphere climate model. Part II. The oceanic circulation. *Journal of Physical Oceanography* 1975; **5**:30–46.
8. Griffies SM. *Fundamentals of Ocean Climate Models*. Princeton University Press: Princeton, NJ, 2004.

9. Zalesak ST. Fully multidimensional flux-corrected transport algorithms for fluids. *Journal of Computational Physics* 1979; **31**:335–362.
10. Gerdes R, Koberle C, Willebrand J. The influence of numerical advection schemes on the results of ocean general circulation models. *Climate Dynamics* 1991; **5**:211–226.
11. Smolarkiewicz PK. A fully multidimensional positive definite advection transport algorithm with small implicit diffusion. *Journal of Computational Physics* 1984; **54**:325–362.
12. Margolin LG, Smolarkiewicz PK. Antidiffusive velocities for multipass donor cell advection. *SIAM Journal on Scientific Computing* 1998; **20**:907–929.
13. Smith RD, Kortas S, Meltz B. Curvilinear coordinates for global ocean models. *Los Alamos National Laboratory Report LAUR-95-1146*, Los Alamos National Laboratory: Los Alamos, NM, 1995.
14. Murray RJ. Explicit generation of orthogonal grids for ocean models. *Journal of Computational Physics* 1996; **126**:251–273.
15. Bleck R, Sun S. Diagnostics of the oceanic thermohaline circulation in a coupled climate model. *Global and Planetary Change* 2003; **40**:233–248.
16. Hasumi H, Suginohara N. Sensitivity of a global ocean general circulation model to tracer advection schemes. *Journal of Physical Oceanography* 1999; **29**:2730–2740.
17. Griffies SM, Pacanowski RC, Hallberg RW. Spurious diapycnal mixing associated with advection in a *z*-coordinate ocean model. *Monthly Weather Review* 2000; **128**:538–564.
18. Yamanaka Y, Furue R, Hasumi H, Suginohara N. Comparison of two classical advection schemes in a general circulation model. *Journal of Physical Oceanography* 2000; **30**:2439–2451.
19. Oschlies A. An unrealistic high-salinity tongue simulated in the tropical Atlantic: another example illustrating the need for a more careful treatment of vertical discretizations in ogcm. *Ocean Modelling* 2000; **1**:101–109.
20. Oschlies A. Equatorial nutrient trapping in biogeochemical ocean models: the role of advection numerics. *Global Biogeochemical Cycles* 2000; **14**:655–667.
21. Najjar RG, Sarmiento JL, Toggweiller JR. Downward transport and fate of organic matter in the ocean. *Global Biogeochemical Cycles* 1992; **6**:45–76.
22. Bleck R. An oceanic general circulation model framed in hybrid isopycnic-cartesian coordinates. *Ocean Modelling* 2002; **37**:55–88.
23. Williams GP. Friction term formulation and convective instability in a shallow atmosphere. *Journal of the Atmospheric Sciences* 1972; **29**:870–876.
24. Gill AE. *Atmosphere-Ocean Dynamics*, International Geophysics Series, vol. 30. Academic Press: San Diego, CA, 92101, 1982.
25. Bleck R, Smith L. A wind-driven isopycnic coordinate model of the north and equatorial atlantic ocean. 1. Model development and supporting experiments. *Journal of Geophysical Research* 1990; **95C**:3273–3285.
26. Killworth PD, Stainforth D, Webb DJ, Paterson SM. The development of a free-surface Bryan–Cox–Semtner ocean model. *Journal of Physical Oceanography* 1991; **21**:1333–1348.
27. Dukowicz JK, Smith RD. Implicit free-surface method for the Bryan–Cox–Semtner ocean model. *Journal of Geophysical Research* 1994; **99**:7991–8014.
28. Higdon RL, de Szoeke RA. Barotropic-baroclinic time splitting for ocean circulation modeling. *Journal of Computational Physics* 1997; **135**:30–53.
29. Bleck R, Boudra D. Wind-driven spin-up in eddy-resolving ocean models formulated in isopycnic and isobaric coordinates. *Journal of Geophysical Research* 1986; **91C**:7611–7621.
30. Farrow DE, Stevens DP. A new tracer advection scheme for Bryan and Cox type ocean general circulation models. *Journal of Physical Oceanography* 1995; **25**:1731–1741.
31. Hecht MW, Holland WR, Rasch PJ. Upwind-weighted advection schemes for ocean tracer transport: an evaluation in a passive tracer context. *Journal of Geophysical Research* 1995; **100**:20763–20778.
32. Stommel H. The westward intensification of wind-driven ocean currents. *Transactions*, *American Geophysical Union* 1948; **29**:202–206.
33. Smolarkiewicz PK. The multi-dimensional Crowley advection scheme. *Monthly Weather Review* 1982; **110**: 1968–1983.
34. Leonard BP. A stable and accurate convective modelling procedure based on quadratic upstream interpolation. *Computer Methods in Applied Mechanics and Engineering* 1979; **19**:59–98.
35. Holland WR, Bryan FO, Chow JC. Application of a third-order upwind scheme in the NCAR Ocean model. *Journal of Climate* 1998; **11**:1487–1493.
36. Hecht MW, Wingate BA, Kassis P. A better, more discriminating test problem for ocean tracer transport. *Ocean Modelling* 2000; **2**:1–15.
37. Webb DJ, deCuevas BA, Richmond CS. Improved advection schemes for ocean models. *Journal of Atmospheric and Oceanic Technology* 1998; **15**:1171–1187.
38. Pacanowski RC. MOM 2 documentation user's guide and reference manual version 1.0. *GFDL Ocean Group Technical Report 3*, Geophys. Fluid Dyn. Lab., Princeton, NJ, 1995.
39. Hecht MW, Bryan FO, Holland WR. A consideration of tracer advection schemes in a primitive equation ocean model. *Journal of Geophysical Research* 1998; **103**:3301–3321.

40. Hunsdorfer W, Trompert RA. Method of lines and direct discretization: a comparison for linear advection. *Applied Numerical Mathematics* 1994; **13**:469–490.
41. Smolarkiewicz PK, Grabowski WW. The multidimensional positive definite advection transport algorithm: nonoscillatory option. *Journal of Computational Physics* 1990; **86**:355–375.
42. Press WH, Flannery BP, Teukolsky SA, Vetterling WT. *Numerical Recipes*. Cambridge University Press: Cambridge, England, 1986.
43. Danabasoglu G, McWilliams JC, Large WC. Approach to equilibrium in accelerated global oceanic models. *Journal of Climate* 1996; **9**:1092–1110.
44. Danabasoglu G. A comparison of global ocean general circulation model solutions obtained with synchronous and accelerated methods. *Ocean Modelling* 2004; **7**(3–4):323–341.
45. Nadiga BT, Hecht MW, Margolin LG, Smolarkiewicz PK. On simulating flows with multiple time scales using a method of averages. *Theoretical and Computational Fluid Dynamics* 1997; **9**:281–292.
46. Smolarkiewicz PK, Margolin LG. On forward-in-time differencing for fluids: extension to a curvilinear framework. *Monthly Weather Review* 1993; **121**:1847–1859.
47. Milliff RF, McWilliams JC. The evolution of boundary pressure in ocean basins. *Journal of Physical Oceanography* 1994; **24**:1317–1338.
48. Grabowski WW, Smolarkiewicz PK. A multiscale anelastic model for meteorological research. *Monthly Weather Review* 2002; **130**(4):939–956.
49. Dubois T, Jauberteau F, Temam RM, Tribbia J. Multilevel schemes for the shallow water equations. *Journal of Computational Physics* 2005; **207**(2):660–694.
50. Reisner J, Wynne S, Margolin L, Linn R. Coupled atmospheric-fire modeling employing the method of averages. *Monthly Weather Review* 2000; **128**:3683–3691.
51. Smolarkiewicz PK, Margolin LG. On forward-in-time differencing for fluids: an Eulerian/semi-Lagrangian non-hydrostatic model for stratified flows. *Atmosphere-Ocean Special* 1997; **35**:127–152.
52. Smolarkiewicz PK, Margolin LG, Wyszogrodski AA. A class of nonhydrostatic global models. *Journal of the Atmospheric Sciences* 2001; **58**:349–364.
53. Warn-Varnas A, Chin-Bing SA, King DB, Smolarkiewicz P, Salusti E, Piacsek S, Hawkins J. Gulf of Gioia ocean-acoustic soliton predictions and studies. *Proceedings of 17th International Congress on Acoustics*, Rome, Italy, September 2001. International Commission for Acoustics; 74–75.
54. Baines PG, Hughes RL. Western boundary current separation: inferences from a laboratory experiment. *Journal of Physical Oceanography* 1996; **26**:2576–2588.
55. Smolarkiewicz PK, Margolin LG. *Implicit Large Eddy Simulation*: *Capturing the Turbulent Flow Dynamics*, Grinstein FF, Margolin L, Rider W (eds), Studies in Geophysics, Chapter 16. Cambridge University Press: Cambridge, U.K., 2005, in preparation.
56. Bleck R. An isentropic coordinate model suitable for lee cyclogenesis simulation. *Rivista di Meteorologia Aeronautica* 1984; **44**:189–194.
57. Benjamin SG, Grell GG, Brown JM, Smirnova TG. Mesoscale weather prediction with the RUC hybrid isentropic-terrain-following coordinate model. *Monthly Weather Review* 2004; **132**:473–494.
58. Drange H, Bleck R. Multidimensional forward-in-time upstream-in-space differencing for fluids. *Monthly Weather Review* 1997; **125**:616–630.
59. Hallberg R, Gnanadesikan A. The role of eddies in determining the structure and response of the wind-driven southern hemisphere overturning: initial results from the modeling eddies in the southern ocean project. *Journal of Physical Oceanography* 2005, under review.
60. Easter RC. Two modified versions of Bott's positive-definite numerical advection scheme. *Monthly Weather Review* 1993; **121**:297–304.
61. de Szoeke RA, Springer SR, Oxilia DM. Orthobaric density: a thermodynamic variable for ocean circulation studies. *Journal of Physical Oceanography* 2000; **30**(11):2830–2852.
62. Higdon RL. A two-level time-stepping method for layered ocean circulation models. *Journal of Computational Physics* 2002; **177**:59–94.
63. Chassignet EP, Smith LT, Bleck R, Bryan FO. A model comparison: numerical simulations of the North and equatorial Atlantic oceanic circulation in depth and isopycnic coordinates. *Journal of Physical Oceanography* 1996; **26**:1849–1867.
64. Halliwell G. Simulation of North Atlantic decadal/multi-decadal winter SST anomalies driven by basin-scale atmospheric circulation anomalies. *Journal of Physical Oceanography* 1998; **28**:5–21.
65. Willebrand J, Barnier B, Böning CW, Dieterich C, Killworth PD, LeProvost C, Jia Y, Molines JM, New AL. Circulation characteristics in three eddy-permitting models of the North Atlantic. *Progress in Oceanography* 2001; **48**:123–161.
66. Sun S, Bleck R. Thermohaline circulation studies with an isopycnic coordinate ocean model. *Journal of Physical Oceanography* 2001; **31**:2761–2782.
67. Houghton JT, Ding Y, Griggs DJ, Noguer M, van der Linden PJ, Dai X, Maskell K, Johnson CA (eds). *Climate Change 2001*: *The Scientific Basis*. Chapter Contribution of Working Group I to the 3rd assessment report of the Intergov. Panel on Climate Change. Cambridge University Press: Cambridge, New York, 2001; 881.

68. Oberhuber JM. Simulation of the Atlantic circulation with a coupled sea ice-mixed layer-isopycnal general circulation model. Part I: model description. *Journal of Physical Oceanography* 1993; **23**:808–829.
69. Sun S, Bleck R. Atlantic thermohaline circulation and its response to increasing CO_2 in a coupled atmosphere-ocean model. *Geophysical Research Letters* 2001; **28**:4223–4226.
70. Sun S, Bleck R. Multi-century simulations with the coupled GISS-HYCOM climate model: control experiments. *Climate Dynamics* 2005, in press.
71. Bleck R, Boudra D. Initial testing of a numerical ocean circulation model using a hybrid (quasi-isopycnic) vertical coordinate. *Journal of Physical Oceanography* 1981; **11**:755–770.
72. Hirt CW, Amsden AA, Cook JL. An arbitrary Lagrangian-Eulerian computing method for all flow speeds. *Journal of Computational Physics* 1974; **14**:227–253.
73. Higdon RL. A two-level time-stepping method for layered ocean circulation models: further development and testing. *Journal of Computational Physics* 2005; **206**:463–504.
74. Dukowicz JK. Structure of the barotropic mode in layered ocean models. *Ocean Modelling* 2005; **11**:49–68.
75. Margolin LG, Shashkov M. Second-order sign-preserving conservative interpolation (remapping) on general grids. *Journal of Computational Physics* 2003; **184**:266–298.

