Upwind-weighted advection schemes for ocean tracer transport: An evaluation in a passive tracer context

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Abstract. Centered-in-space, centered-in-time integration has generally been used for the advection of scalars in ocean models. An assessment is made of the implications of centered leapfrog integration in the context of two-dimensional passive tracer advection within a Stommel (1948) gyre. Nonphysical ripples in the tracer field grow to alarming levels in purely advective integrations. Diffusive parameterizations of eddy mixing moderate these ripples, but it is found that Laplacian diffusion greatly reduces the peak amplitude of the tracer field, whilebiharmonic or weaker Laplacian diffusion allows ripples of large amplitude. Several forward-in-time, upwind-weighted schemes are found to provide better solutions. Smolarkiewicz's (1984) Multi-Dimensional Positive-Definite Advection and Transport Algorithm (MPDATA) scheme is slightly superior for an integration at moderate resolution within which the western boundary current is poorly resolved in typical fashion. Third-order, upwind-based schemes exhibit little sensitivity to the details of multidimensional treatment for this problem of passive tracer advection, with results nearly as good as for MPDATA.

1. Introduction

The evolution of two of the five prognostic variables in a typical ocean model (e.g., the primitive equation model of Bryan and Cox [Bryan, 1969, Cox, 1948]) is determined by the numerical treatment of the tracer transport equation. The vast majority of ocean models discretize the tracer transport equation with centered spatial differencing and centered-in-time or leapfrog temporal treatment. The efficiency, simplicity of implementation, and \( O(\Delta x^2) \) accuracy of centered differencing are largely responsible for this wide usage.

The dispersive nature of centered differencing makes it inappropriate for application to purely advective problems. Eddy mixing is parameterized by Laplacian or biharmonic diffusion in ocean models, and so transport is described by an advection/diffusion equation. The diffusion moderates the rippling of the tracer fields induced by the centered differencing. It might even be said that the magnitude of the diffusion is dictated by smoothness of solutions rather than physical considerations. Ripples in the tracer fields may generally be expected to persist unless the strength of the diffusion is raised to levels which largely negate the \( O(\Delta x^2) \) accuracy of the centered differencing, as we demonstrate in this paper.

Ripples in the tracer fields sometimes grow to become nonphysical extrema which may be readily identified. Gerdes et al. [1991] discuss such a nonphysical maximum in a model salinity field near the equator which is associated with a physical minimum nearby. Numerical errors in the density field may destabilize the dynamics. In a parameter sensitivity study, Bryan [1987] found an anomalous deep equatorial cell in the meridional mass transport stream function when the vertical diffusivity was reduced from \( 5 \times 10^{-5} \) to \( 1 \times 10^{-5} \text{ m}^2 \text{s}^{-1} \) which may be the result of an instability of the centered differencing scheme at this low but possibly realistic value of the vertical diffusivity [Ledwell et al., 1993; Toole et al., 1994]. More recently, Farrow and Stevens [1995] document large excursions in the temperature field at the confluence of the Brazil and Malvinas currents which are associated with the centered differencing in the United Kingdom fine resolution Antarctic model.

Forward-in-time, upwind-weighted schemes offer a less dispersive alternative to leapfrog. These schemes have been widely adopted in computational fluid dynamics for the solution of flux form equations. Upwind-weighted schemes have, in fact, seen little application in ocean modeling. The implementation of flux corrected transport in a Geophysical Fluid Dynamics Laboratory (GFDL) model of Gerdes et al. [1991] combined donor cell upwind differencing with centered differencing with an early form of flux limitation outlined by Zalesak [1979]. They document the disappearance of the nonphysical extremum mentioned above when they use upwind-weighted differencing. Farrow and Stevens [1995] have implemented the Quadratic Upstream Interpolation for Convective Kinematics (QUICK) scheme of Leonard [1979] which is \( O(\Delta x^2) \) in the limit of a
uniform flow field. They report the disappearance of anomalous temperature excursions with the upwind-weighted scheme. We have implemented the fully three-dimensional Multi-Dimensional Positive-Definite Advection and Transport Algorithm (MPDATA) scheme of Smolarkiewicz [1984] and the QUICK with Estimated Streaming Terms (QUICKEST) scheme of Leonard [1979] in a GFDL model. Comparisons with centered differencing will be documented in the literature.

Intense boundary flow with strong shear is one characteristic problem facing ocean models. In this paper we evaluate centered differencing and several upwind-weighted schemes applied to two-dimensional passive tracer transport where the flow field is the western boundary intensified gyre of Stommel [1948]. Schemes under consideration include $O(\Delta x)$ donor cell upwind differencing, several implementations based on the higher-order upwind differencing scheme known as QUICKEST [Leonard, 1979], Smolarkiewicz's [1984] fully multidimensional MPDATA, and a monotonic scheme of van Leer [1974], (also see Allen et al. [1991]). The application of explicit diffusion to moderate rippling is studied. The effect of nonuniform grid spacing is also investigated. In place of an analytic solution to the problem we use an analytic expression for the velocity field to obtain a Lagrangian reference solution for the purely advective case through numerical integration of the trajectories backward in time from each arrival point. The validity of this reference solution is confirmed through a scaling analysis which is discussed in the appendix.

This research has been pursued in response to the problematic rippling produced by centered differencing, and yet we are not of the opinion that rippling of any degree is intolerable. Mild rippling is readily suppressed by explicit diffusion in most modeling applications, and therefore we consider forms of the QUICKEST-based schemes and MPDATA without flux correction. Examples of flux limitation applied to those schemes are given by Leonard [1991], Leonard et al. [1993], and Smolarkiewicz and Grubowski [1990].

In section 2 the nature of the numerical experiment is outlined. Section 3 discusses the implementation of forward-in-time, upwind-weighted schemes. Results are presented in section 4 and some concluding statements appear in section 5.

2. Experiment

The oceanic advection of heat and salt involves the transport of anomalies in the tracer fields. We pose the problem of accurate advection of an anomaly in a tracer field through a Stommel [1948] gyre. The particular anomaly chosen is a Gaussian of width 800 km and amplitude of 1.0 which is applied above a background tracer value of 1.0. All of the figures and error analysis presented in this paper treat only the anomaly in the tracer field after subtraction of the background tracer value of 1.0.

2.1. Continuum Description

The flow field is the beta-plane solution for wind-driven western boundary intensified basin circulation of Stommel [1948]. The parameters Stommel used yield a western boundary current of reasonable width (around 100 km), and so we use exactly those same parameters. The mass transport stream function is

$$\Psi = D\gamma(\frac{b}{\pi})^{2}\sin(\frac{\pi y}{b})(p\exp A\eta + q\exp B\eta) - 1$$

where the zonal extent of the basin is $\lambda = 10^4$ km; the meridional extent is $b = 2\pi \times 10^6$ km; and the depth, applied wind stress, frictional coefficient, and Coriolis parameter are $D=200$ m, $F=0.1$ N m$^{-2}$, $R = 0.02$, and $f = y \times 10^{-11}$ m$^{-1}$ s$^{-1}$, respectively.

In (1),

$$\gamma = \frac{F\pi}{Rb}$$

$$\alpha = \frac{D \partial f}{R \partial y}$$

$$A = -\alpha/2 + [\alpha^2/4 + (\pi/b)^2]^{1/2}$$

$$B = -\alpha/2 - [\alpha^2/4 + (\pi/b)^2]^{1/2}$$

$$p = (1 - \exp B\lambda)/(\exp A\lambda - \exp B\lambda)$$

$$q = 1 - p.$$
in the western boundary region are more than an order of magnitude greater than typical velocities throughout the rest of the domain. The maximum northward velocity of 2.19 m s\(^{-1}\) is found at \(x = 0\). In contrast, the maximum southward velocity is only 0.025 m s\(^{-1}\).

The reference solution at five evenly spaced intermediate times and at the final time is seen in Figure 2. The challenge facing the candidate advection schemes of reproducing this flow through a fast boundary current which is poorly resolved may be appreciated, particularly from Figures 2b and 2c, where the tracer anomaly is passing through the boundary flow.

### 2.2. Discretization

The finite difference velocity field to be used below is calculated through finite differencing of (1) for the stream function so that the velocity satisfies the discretized equation of continuity. An Arakawa B grid [Arakawa and Lamb, 1977] is used, as in the GFDL model, so that velocities are known on a grid which is staggered relative to that of the tracers and the stream function. All of the advective schemes (including the centered scheme) require velocities at the faces of the tracer cells in order to compute fluxes through those faces. These face-centered velocities are derived from weighted averages of pairs of velocities, as in the GFDL model [Bryan, 1969].

We discretize the domain with 100 km grid spacing for experiments on the regular grid, and for most experiments on an irregular or stretched grid we use the same meridional grid spacing with a variable zonal grid spacing which retains the same number of grid elements.

![Figure 2](image-url)

**Figure 2.** Reference solutions derived from a Runge Kutta integration of the analytic velocity field at (a) \(2.5 \times 10^7\), (b) \(5 \times 10^7\), (c) \(7.5 \times 10^7\), (d) \(10^8\), (e) \(1.25 \times 10^8\), and (f) \(1.5 \times 10^8\) s.
Velocity points define the boundaries, while stream function and tracer points straddle those boundaries. The boundary velocities are constrained to have no normal component. Stream function values just outside the boundary are set equal in magnitude to their nearest neighbor just inside the boundary but with opposite sign in order to satisfy this constraint. The advection schemes require one or two rows of tracer points outside of the boundaries. These extra rows of tracer points are filled by setting them equal to their nearest neighbor inside the domain.

The choice of time step is discussed in section 4. All analysis is done at a final time of $1.5 \times 10^8$ s (see Figure 2f), after approximately 5 years of simulated time, at which point the initial anomaly has been advected through the western boundary current but has not yet begun a second pass through the western boundary current.

3. Upwind-Weighted Schemes

The leading truncation error from upwind differencing is of the form of a diffusive term, Laplacian for $O(\Delta x)$ donor cell upwind differencing and biharmonic for $O(\Delta x^3)$ upwind differencing. Upwind-weighted schemes are generally implemented in a forward-in-time sense for reasons of stability, as one might expect from the lack of stability of the diffusion and biharmonic dissipation equations under centered-in-time treatment (see Rosche [1976] or Leonard [1979] for stability analyses of some upwind-weighted schemes).

The transport equation, with $R$ representing any non-advection terms,

$$\frac{\partial T}{\partial t} + \nabla \cdot (uT) = R$$

may be discretized in a forward-in-time sense as

$$\frac{T^{n+1} - T^n}{\Delta t} + \nabla \cdot (u^{n+1/2}T^n) = R^{n+1/2}. \quad (9)$$

Fully multidimensional advection schemes such as MPDATA and UTOPIA treat the flux-form operator $\nabla \cdot (u^{n+1/2}T^n)$ in such a way that (8) is recovered from a Taylor's series analysis to second-order accuracy. When applying one-dimensional advection schemes such as QUICKEST and the van Leer [1974] scheme to multidimensional flow, care must be taken in order to represent (8) to second-order accuracy.

3.1. Operator Split Implementation of One-Dimensional Schemes

As a recipe for the implementation of a forward-in-time, upwind-weighted scheme in an ocean model, one must first choose a particular multidimensional scheme or a one-dimensional scheme. If a one-dimensional scheme is chosen (presumably for reasons of computational efficiency), the stability properties of the one-dimensional scheme will be retained in more than one dimension if operator splitting is applied. Operator splitting of a forward-in-time, one-dimensional advection scheme for higher-dimensional flow will break second-order accuracy through the failure to reproduce cross terms arising between dimensions. However, Strang [1968] found that these cross terms are recovered after two time steps if one operator splits with alternating directions in two dimensions.

In the case of transport in two dimensions one advects first in one direction, producing an intermediate solution $T(\alpha)$, and then the intermediate solution is advected in the second direction, as

$$T(\alpha) = T(n) + \Delta t \text{ADV}[T(n), u_i(n + \frac{1}{2})] \quad (10a)$$

$$T(n + 1) = T(\alpha) + \Delta t \text{ADV}[T(\alpha), u_i(n + \frac{1}{2})] \quad (10b)$$

where ADV represents the one-dimensional advection operator of the chosen scheme. For the case of spatially uniform flow the resulting solution after two time steps is equivalent to a fully multidimensional solution to second-order accuracy.

An independent error arises when the flow field is not spatially uniform. This error, which is proportional to the gradient of the velocity may be identified through a Taylor's series analysis, as in the work by Smolarkiewicz [1991], and may be compensated through advection with $U$ in place of $u$ in (10a) and (10b), where

$$u_i = u_i(n + \frac{1}{2}) - \frac{\Delta t}{2} u_i(n) \partial u_i(n)/\partial x_i. \quad (11)$$

We apply operator splitting with alternating directions in order to cancel the errors arising from the splitting, and we advect with $U$ in place of $u$ in order to cancel the error terms which are proportional to the velocity gradient. The resulting procedure is written as

$$T(\alpha) = T(n) + \Delta t \text{ADV}[T(n), U_i] \quad (12a)$$

$$T(n + 1) = T(\alpha) + \Delta t \text{ADV}[T(\alpha), U_i]. \quad (12b)$$

The midpoint velocity $u_i[n + (1/2)]$ is computed with interpolation if possible or with extrapolation (the relative magnitude of the truncation error will depend on the method of estimation). One may incorporate diffusion at $O(\Delta t)$ by including a diffusive operator $D$ evaluated at time step $n$ on the right-hand side of (9).

Hundsdorfer and Tromperr [1994] discuss both of these error terms and their compensation in very clear terms and also offer an alternative to the method of alternating directions for two-dimensional flow. We have extended their analysis from two to three dimensions and have compensated the splitting errors without alternating directions in a three-dimensional application of QUICKEST to tracer advection in a GFDL ocean model. This work will be discussed in a forthcoming manuscript.

3.2. The Schemes

Centered-in-space, centered-in-time integration is compared with donor cell upwind differencing, several forms
based on QUICKST, Smolarkiewicz's [1984] MPDATA, and a van Leer [1974] scheme. Donor cell upwind differencing [Roache, 1976] is the only one of the schemes which is of only $O(\Delta x)$ accuracy. It is a simple, monotonic alternative to $O(\Delta x^2)$ centered differencing.

Smolarkiewicz' s [1984] MPDATA is a fully multidimensional scheme which is applied in an iterative manner. The first iteration produces $O(\Delta x)$ donor cell upwind differencing. The second, "antidiffusive," iteration raises the result to $O(\Delta x^2)$ accuracy. Further iterations may be used. We apply only two iterations (one anti-diffusive iteration).

The one-dimensional QUICKST scheme is used in operator split form, both with and without compensation of the velocity gradient error term, in the forms described by (10a), (10b), (12a), and (12b). A fully two-dimensional implementation referred to as UTOPIA is also used [Leonard et al., 1993]; we use the particular stencil and form of Rasch [1994].

A van Leer [1974] scheme provides a relatively simple, monotonic, one-dimensional advection scheme. We operator split the scheme, compensating the error term arising from the spatial variability of the flow field, as with QUICKST. We note that the monotonicity is broken by the operator split implementation.

The schemes are referred to as centered-in-time, centered-in-space (CTCS), donor cell ($O(\Delta x)$ upwind differencing), MPDATA, QUICKST (operator split, with compensation of the velocity gradient error term unless otherwise noted), UTOPIA (fully two-dimensional implementation of QUICKST), and van Leer [van Leer, 1974]. The schemes are listed in Table 1, along with references.

Our implementations of these schemes were not optimized for computational efficiency. With this caveat we present cost factors. We define the cost factor as the CPU time per time step, normalized to the cost of two steps of the CTCS scheme (it requires two steps of centered leapfrog to get as far as with one forward-in-time step at the same Courant number). The cost factors are 2.6 for MPDATA, 1.6 for UTOPIA, 1.1 for QUICKST, 1.9 for van Leer, and 0.6 for donor cell. All timings were done on a Sun SPARCstation 10.

4. Results

Results of advection with the different schemes are presented for visual inspection in Figures 2-10. Error measures are also presented for more quantitative comparison. Error measures in the form proposed by Williamson [1992] are used.

All error measures are computed in terms of the anomaly in the tracer field. If the anomaly is represented by $T$,

$$T(i,j) = T(i,j) - 1$$  \hspace{1cm} (13)

$T_r$ is the reference solution and $[f(i,j)]$ is the area weighted average of $f(i,j)$,

$$[f(i,j)] = \sum_{i,j} \Delta x(i) \Delta y(j) f(i,j)$$  \hspace{1cm} (14)

then the error measures are

$$l_1 = \frac{I\{T(i,j) - T_r(i,j)\}}{I\{T_r(i,j)\}}$$  \hspace{1cm} (15)

for the $l_1$ error measure, and

$$l_2 = \frac{\sqrt{\left[I\{(T(i,j) - T_r(i,j))^2\}\right]}}{\sqrt{\left[I\{T_r(i,j)\}\right]}}$$  \hspace{1cm} (16)

for the second moment $l_2$ of the error field. The $l_1$ error measure is something like a first moment of the error field and would be exactly so were it not for the absolute value operations which are applied. A measure of the maximum departure of the candidate solution from the reference solution is $l_\infty$,

$$l_\infty = \max_{i,j} \frac{[T(i,j) - T_r(i,j)]}{[T_r(i,j)]}.$$  \hspace{1cm} (17)

The variance is

$$V = \frac{\left[I\{(T(i,j) - I\{T(i,j)\})^2\}\right]}{\left[I\{T_r(i,j) - I\{T_r(i,j)\}\}\right]} - 1$$  \hspace{1cm} (18)

<table>
<thead>
<tr>
<th>Table 1. The Advection Schemes</th>
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<tbody>
<tr>
<td>Scheme</td>
</tr>
<tr>
<td>CTCS</td>
</tr>
<tr>
<td>MPDATA</td>
</tr>
<tr>
<td>UTOPIA</td>
</tr>
<tr>
<td>QUICKST</td>
</tr>
<tr>
<td>van Leer</td>
</tr>
<tr>
<td>Donor cell</td>
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</table>


and error measures in the determination of minimum and maximum values in the anomaly field are

$$\text{MIN} = \min_{V_{i,j}} [T(i,j)] - \min_{V_{i,j}} [T_r(i,j)]$$  \hspace{1cm} (19)

$$\text{MAX} = \max_{V_{i,j}} [T(i,j)] - \max_{V_{i,j}} [T_r(i,j)]$$  \hspace{1cm} (20)

The usefulness of the error measures depends on the precision of the reference solution which is numerically obtained from the analytic form for the velocities. In the appendix we show that the error measures converge steadily and predictably when we compare a finite difference based solution at several resolutions to the numerically derived reference solution. This convergence of finite difference solution and numerical reference solution validates the accuracy of the reference solution.

4.1. Pure Advection on Regular Grid

We first consider the problem of pure advection on a regular grid. On this grid the maximum velocity is 1.72 m s$^{-1}$. All of the schemes are well behaved at Courant numbers approaching 1 under these purely advective conditions. We perform these integrations with a time step of $5.0 \times 10^4$ s, where the maximum Courant number is 0.86. We use 1/2 of this time step for the centered-in-space, centered-in-time integration since the tracer field is stepped through $2\Delta t$ with the three time level leapfrog integration.

A sequence of six snapshots taken at uniform intervals is presented for centered differencing (CTCS) in Figure 3. The dramatic convergence of streamlines causes the tracer distribution to pass within the narrow western boundary current. The intense flow through the bound-

![Figure 3](image-url)

**Figure 3.** Snapshots taken at uniform intervals of simulated time, with centered-in-time, centered-in-space (CTCS) differencing at (a) $2.5 \times 10^7$, (b) $5 \times 10^7$, (c) $7.5 \times 10^7$, (d) $10^8$, (e) $1.25 \times 10^8$, and (f) $1.5 \times 10^8$ s.
arated upwind differencing is the simplest alternative we consider to centered differencing. The diffusive nature of the scheme is immediately apparent in Figure 6b. The scheme is monotonic, and hence there are no undershoots (MIN = 0 in Table 2), but the preservation of peak amplitude is very poor (the MAX error measure indicates a 79% loss of peak amplitude). Integration with donor cell upwind differencing approaches a perfect solution as the Courant number approaches one. The highly nonuniform nature of oceanic circulations (that is, the Courant number varies strongly from place to place and from time to time) makes donor cell upwind differencing a poor choice for ocean modeling.

All of the higher-order, upwind-weighted schemes show good shape preservation and much reduced rippling which is reflected in the much more moderate MIN errors. QUICKEST and the fully two-dimensional UTOPIA, in particular, are nearly indistinguishable, suggesting that the fully two-dimensional and the operator split implementations of QUICKEST (following the form of (10a) and (10b)) are nearly equivalent for our test problem. We also include the uncompensated form of QUICKEST (following (12a) and (12b)). This form is comparable to the compensated form and to UTOPIA in all error measures except for the tendency to produce downward ripples in the tracer field, reflected in a larger MIN error.

The van Leer scheme trails all of the other higher-order, forward-in-time schemes in all error measures except for the error in the minimum value. Although operator splitting has broken the monotonicity, the split scheme is still nearly monotonic. This scheme is not ideal for use in all three dimensions of an ocean model due to the relatively large errors. In the case of biogeochemical modeling, where monotonicity at least in the vertical dimension may be required, the van Leer scheme may be a good candidate for treating that one dimension, splitting the scheme with one of the other forward-in-time schemes in the horizontal dimensions.

The error measures for MPDATA are superior for all but the minimum, although the differences are relatively small. For instance, the second moment of the error field $l_2$ is about 10% smaller for MPDATA than for the three QUICKEST-based schemes. The error in the minimum is greater than that of the other upwind-weighted schemes (except for the uncompensated version of QUICKEST) but is an order of magnitude smaller than that of the centered-differencing (CTCS) scheme. We conclude that MPDATA is slightly superior for use with highly sheared and poorly resolved flows, as in this test case and as in much of ocean modeling.

The error measures for CTCS are inferior to those of the upwind-weighted schemes except in the case of the variance. This superior tendency to preserve the variance may also be expected to be reduced or even reversed when tested in an ocean model. The rippling

| Table 2. Error Measure on Regular Grid 1° Resolution |
|-----------------|--------|--------|--------|--------|--------|--------|
| Scheme          | MIN    | MAX    | $l_1$  | $l_2$  | $l_{oo}$| $V$    |
| CTCS            | -0.64  | -0.31  | 1.14   | 0.68   | 0.67   | 0.01   |
| MPDATA          | -0.09  | -0.45  | 0.72   | 0.50   | 0.46   | -0.47  |
| UTOPIA          | -0.04  | -0.49  | 0.78   | 0.57   | 0.54   | -0.53  |
| QUICKEST        | -0.04  | -0.49  | 0.80   | 0.57   | 0.54   | -0.53  |
| QUICKEST,       |        |        |        |        |        |        |
| uncompensated   | -0.11  | -0.46  | 0.91   | 0.56   | 0.52   | -0.46  |
| van Leer [1974] | -0.01  | -0.64  | 0.94   | 0.67   | 0.65   | -0.64  |
| Donor cell      | 0.0    | -0.79  | 1.16   | 0.78   | 0.80   | -0.81  |

Abbreviations are defined as follows: MIN, minimum value in the anomaly field; MAX, maximum value in the anomaly field; $l_2$, second moment of the error field; $l_{oo}$, maximum departure of the candidate solution from the reference solution; and $V$, variance. The $l_1$ error measure resembles a first moment of the error field, as discussed in Section 4.
of the tracer fields produced by the scheme generates enhanced gradients. The resulting diffusion will reduce the variance. Farrow and Stevens [1995] noted such a net loss of variance for centered differencing relative to the upwind-weighted QUICK scheme. We record similar results when we examine the advection/diffusion problem section 4.2.

### 4.2. Advection and Diffusion on Regular Grid

Ocean modeling is not a purely advective problem. In either the horizontal plane or within isopycnal surfaces we parameterize eddy mixing through diffusion. This diffusion moderates the rippling seen in section 4.1. Even in the vertical direction, a small diffusivity is included which represents slow diapycnal diffusion and moderates the ripples produced in the much weaker vertical component of the circulation.

We refer to biharmonic dissipation as diffusion, as is conventional in ocean modeling. In other contexts one would consider a diffusive term to be of Laplacian form and a term of biharmonic form would be referred to as dissipative.

There is evidence that the diffusion used in ocean models is not always sufficient to suppress ripples in the tracer fields, as noted in section 1. If it is chosen to be large enough to suppress ripples, then it is unrealis-
Figure 5. Snapshots taken at uniform intervals of simulated time with QUICKEST (operator split, as in (12a) and (12b)) at (a) $2.5 \times 10^7$, (b) $5 \times 10^7$, (c) $7.5 \times 10^7$, (d) $10^8$, (e) $1.25 \times 10^8$, and (f) $1.5 \times 10^8$ s.

An ocean model at around 1° will typically be run with a Laplacian diffusivity of around $2 \times 10^3$ m$^2$ s$^{-1}$ [Böning et al., 1994]. The net effect is strikingly similar to that from donor cell upwind differencing, as seen in a visual comparison of Figures 7a and 6h or through the error measures listed in Tables 3 and 2.

A biharmonic diffusivity of $8 \times 10^{13}$ m$^4$ s$^{-1}$ corresponds to the same dissipation time for 2Δx features as does the Laplacian diffusivity of $2 \times 10^3$ m$^2$ s$^{-1}$. The final tracer distribution resulting from integration with this level of biharmonic diffusion is seen in Figure 7c. The peak amplitude of the tracer anomaly (the loss of which is quantified by the MAX error measure) is more comparable to that from the upwind-weighted integrations. Some 2Δx ripples are seen in the contours, and...
Figure 6. Results of pure advection on a regular grid with spacing of 100 km, at the final time of $1.5 \times 10^8$ s for (a) reference solution; (b) centered-in-time, centered-in-space (CTCS); (c) MPDATA; (d) UTOPIA; (e) QUICKEST (operator split, as in (12a) and (12b)); (f) QUICKEST, without compensation of the velocity gradient error term (operator split, as in (10a) and (10b)); (g) van Leer [1974] (operator split, as in (12a) and (12b)); and (h) donor cell upwind differencing.
Figure 7. Solutions of advection/diffusion equations based on centered-in-time, centered-in-space (CTCS) integration of the advective terms at a final time of $1.5 \times 10^8$ s showing (a) Laplacian diffusivity of $2 \times 10^{10}$ m$^2$ s$^{-1}$, (b) Laplacian diffusivity of $1.6 \times 10^2$ m$^2$ s$^{-1}$, (c) biharmonic diffusivity of $8 \times 10^{13}$ m$^4$ s$^{-1}$, and (d) biharmonic diffusivity of $5 \times 10^{13}$ m$^4$ s$^{-1}$.

There are some relatively small downward ripples in the tracer anomaly field which have been contoured and which are quantified by the MIN error measure.

Errors in the maximum value of the anomaly field which are comparable to those from the best of the upwind-weighted integrations were found at a Laplacian diffusivity of $1.6 \times 10^2$ m$^2$ s$^{-1}$, as seen in Figure 7b, and at a biharmonic diffusivity of $5 \times 10^{13}$ m$^4$ s$^{-1}$, as seen in Figure 7d. All of the other error measures at the final time are also comparable between these two diffusive simulations and the purely advective upwind-weighted simulations. In particular, we note that the very much smaller error in the variance ($V$) which was observed for centered differencing (CTCS) in the purely advective experiment has increased greatly with the inclusion of diffusion.

Table 3. Error Measures for Advection/Diffusion Problem on Regular Grid for Centered Leapfrog Integration

<table>
<thead>
<tr>
<th>Diffusivity</th>
<th>MIN</th>
<th>MAX</th>
<th>$l_1$</th>
<th>$l_2$</th>
<th>$l_\infty$</th>
<th>$V$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2 \times 10^{10}$ m$^2$ s$^{-1}$</td>
<td>-0.0</td>
<td>-0.80</td>
<td>1.25</td>
<td>0.82</td>
<td>0.84</td>
<td>-0.83</td>
</tr>
<tr>
<td>$1.6 \times 10^2$ m$^2$ s$^{-1}$</td>
<td>-0.12</td>
<td>-0.47</td>
<td>0.74</td>
<td>0.51</td>
<td>0.48</td>
<td>-0.48</td>
</tr>
<tr>
<td>$8 \times 10^{13}$ m$^4$ s$^{-1}$</td>
<td>-0.08</td>
<td>-0.52</td>
<td>0.85</td>
<td>0.53</td>
<td>0.56</td>
<td>-0.48</td>
</tr>
<tr>
<td>$5 \times 10^{13}$ m$^4$ s$^{-1}$</td>
<td>-0.09</td>
<td>-0.47</td>
<td>0.84</td>
<td>0.51</td>
<td>0.51</td>
<td>-0.42</td>
</tr>
</tbody>
</table>

See Table 2 for definitions.

These error measures at the final time step do little to dissuade one from modeling ocean circulation with small diffusivities. The results at the final time are not the entire story. If we examine Figure 8 for the maximum amplitude of downward ripples as a function of time we find that the two biharmonic simulations and the Laplacian simulation at lower diffusivity produce very large ripples at intermediate times which are dissipated away at later, more quiescent times. Such ripples in the temperature or salinity fields of an ocean model could be expected to feed back strongly on the dynamics. Only the simulation at Laplacian diffusivity of $2 \times 10^{10}$ m$^2$ s$^{-1}$ is free of these ripples, and it is this simulation which looks so similar to the donor cell upwind differencing.

4.3. Pure Advection on Stretched Grid

The resolution of the narrow western boundary current in the Stommel [1948] gyre may be easily improved without using any more grid points due to the high degree of symmetry in the stream function. We use a variable zonal grid spacing which varies smoothly from $0.1 \times \Delta x_{\text{max}}$ to $\Delta x_{\text{max}}$ via a cosine function. The easternmost 40% of the grid elements are of the full size $\Delta x_{\text{max}}$. With the variable zonal grid spacing we cover the westernmost 100 km with seven grid points rather than just one on the regular grid.
Ocean models commonly contain such a dramatically stretched grid, although the extreme stretching is of the vertical coordinate rather than a horizontal coordinate. By stretching the grid in this advective test problem, we not only illuminate the effect of resolution, but also test the schemes on a grid which is stretched to a degree that is roughly comparable to that of a vertical grid in an ocean model. Indeed, if one turns the Stommel [1948] gyre on its side so that the western boundary current appears at the top, the circulation bears some resemblance to a zonally integrated ocean circulation with strong vertical shear in the upper layers.

On the stretched grid the maximum velocity is 2.12 m s⁻¹. Several of the schemes produce stable results at high Courant numbers, however centered differencing (CTCS) begins to produce extreme values as the tracer anomaly is advected through the boundary current at a Courant number of 0.74. This error growth is not observed at a Courant number of 0.64. We run all the forward-in-time, upwind-weighted schemes at a time step of \(4 \times 10^4\) s corresponding to a maximum Courant number of 0.85. For the centered-in-time leapfrog integration (CTCS) we use a time step of \(1.5 \times 10^4\) s (the leapfrog scheme steps through \(2\Delta t\)) corresponding to a Courant number of 0.64.

Much improved results are seen with all of the schemes on the stretched grid in Figure 9, although the importance of \(O(\Delta x^2)\) accuracy is clearly seen when comparing the \(O(\Delta x)\) donor cell upwinding with any of the other algorithms. The slight advantage possessed by MPDATA on the regular grid has been reversed in favor of UTOPIA and QUICKEST now that the flow has been better resolved, as indicated by a comparison of the error measures listed in Table 4.

The errors (of negative sign in some cases, of positive sign in others) which were seen to develop in the northwest corner of all of the integrations on the regular grid (as seen in Figure 6) are absent for all integrations on the stretched grid except for the uncompensated form of QUICKEST (operator split according to (10a) and (10b), as seen in Figure 9f. The error measures listed in Table 4 are much worse for this scheme than for any of the other schemes of second-order accuracy, and it seems apparent that this primarily reflects the erroneous feature which is propagating along the northern boundary from the northwest corner. Whereas we observed little difference between the compensated and uncompensated forms of operator split QUICKEST on the regular grid, it is clear from Figure 9f that compensation of the velocity gradient error term, as in (12a) and (12b), is worthwhile. The basis for this problematic behavior of the uncompensated form of QUICKEST is largely explained by its inability to preserve an initially constant tracer value, as discussed in section 4.4.

The error measures for the van Leer scheme on the stretched grid are uniformly worse than for the other higher-order, forward-in-time schemes, as was also the case on the regular grid. Whereas errors which are primarily diffusive in nature are much reduced for the upwind-weighted schemes on the stretched grid, dispersive errors are much reduced for the centered-in-space, centered-in-time scheme. The stretched grid integrations show us the importance of resolution, and when contrasted with the regular grid integrations, we are reminded of the importance of the advective treatment when flows are poorly resolved.

4.4. Preservation of a Constant

Preservation of a constant scalar value under advection is a desirable quality. When we initialize the tracer field with a constant value and integrate for several time steps in order to test for preservation of a constant, we see an advantage of fully multidimensional schemes over operator split, one-dimensional forms.

The fully multidimensional schemes MPDATA and UTOPIA preserve the initially constant tracer value (to machine precision), as indicated in Table 5. Centered leapfrog (CTCS) and donor cell upwind differencing also preserve an initially constant value.

The operator split implementation of QUICKEST (following (12a) and (12b)) formally approximates UTOPIA to second order. A casualty of this approximation is the preservation of a constant. The uncompensated operator split implementation of QUICK-EST (following (10a) and (10b)) formally approximates UTOPIA only to \(O(1)\), and its violation of the preservation of a constant is greater, especially on the stretched grid, as documented in Table 5. The operator split implementation of the van Leer algorithm also violates the preservation of a constant.

5. Conclusions

The loss of amplitude and reduction in variance is of particular note for all of the upwind-weighted algo-
Figure 9. Results of pure advection on a stretched grid at the final time of $1.5 \times 10^8$ s for (a) reference solution; (b) centered-in-time, centered-in-space; (c) MPDATA; (d) UTOPIA; (e) QUICKEST (operator split, as in (12a) and (12b)); (f) QUICKEST without compensation of the velocity gradient error term (operator split, as in (10a) and (10b)); (g) van Leer [1974] (operator split, as in (12a) and (12b)); and (h) donor cell upwind differencing.
Table 4. Error Measures on Stretched Grid, 1° Resolution

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Courant Number</th>
<th>MIN</th>
<th>MAX</th>
<th>$l_1$</th>
<th>$l_2$</th>
<th>$l_\infty$</th>
<th>V</th>
</tr>
</thead>
<tbody>
<tr>
<td>CTCS</td>
<td>0.64</td>
<td>0.00</td>
<td>0.18</td>
<td>0.13</td>
<td>0.15</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td>MPDATA</td>
<td>0.85</td>
<td>-0.02</td>
<td>-0.12</td>
<td>0.19</td>
<td>0.16</td>
<td>0.20</td>
<td>-0.13</td>
</tr>
<tr>
<td>UTOPIA</td>
<td>0.85</td>
<td>-0.02</td>
<td>-0.11</td>
<td>0.16</td>
<td>0.12</td>
<td>0.11</td>
<td>-0.08</td>
</tr>
<tr>
<td>QUICKEST</td>
<td>0.85</td>
<td>-0.02</td>
<td>-0.10</td>
<td>0.14</td>
<td>0.11</td>
<td>0.10</td>
<td>-0.07</td>
</tr>
<tr>
<td>QUICKEST,</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>uncompensated</td>
<td>0.85</td>
<td>-0.18</td>
<td>-0.07</td>
<td>0.68</td>
<td>0.31</td>
<td>0.18</td>
<td>0.11</td>
</tr>
<tr>
<td>van Leer [1974]</td>
<td>0.85</td>
<td>-0.01</td>
<td>-0.26</td>
<td>0.24</td>
<td>0.20</td>
<td>0.26</td>
<td>-0.18</td>
</tr>
<tr>
<td>Donor cell</td>
<td>0.85</td>
<td>0.0</td>
<td>-0.71</td>
<td>1.03</td>
<td>0.66</td>
<td>0.71</td>
<td>-0.73</td>
</tr>
</tbody>
</table>

See Table 2 for definitions.

algorithms on the uniform grid. However, if we require the ripples in the tracer field to be of no more than moderate amplitude, we find that the error measures for the higher-order, forward-in-time schemes are superior to those for centered-in-space, centered-in-time integration which is moderated with diffusion.

Our first recommendation is to consider a forward-in-time scheme of $O(\Delta x^2)$ or higher. One may expect unphysical extrema to disappear, as supported by the work of Gerdes et al. [1991], Farrow and Stevens [1995], and that presented in this paper. There are bound to be more subtle errors in the dynamics which will disappear along with these errors in the density field. The use of upwind-weighted advection schemes will also allow ocean modelers to experiment with a much wider range of diffusivities than has been possible with centered differencing (CTCS), making possible the use of smaller values that are in better accord with observations.

MPDATA appears to be one good choice. It performs slightly better than the QUICKEST-based schemes on the regular grid, where the highly sheared boundary flow is poorly resolved. This problem of having few grid points in the boundary jet is typical of ocean modeling.

The QUICKEST-based schemes perform nearly as well as MPDATA. The implementation of QUICKEST which includes compensation of the velocity gradient error terms, as in (12a) and (12b), is comparable to the more elaborate, fully two-dimensional implementation of UTOPIA in our tests and is also particularly efficient, as noted in section 2.2. The uncompensated form of QUICKEST (following (10a) and (10b)) is problematic on the stretched grid, and the minor gains of simplicity and efficiency obtained through the avoidance of the calculation of (11) is unjustifiable.

The van Leer scheme does not perform as well as some of the other schemes but may have a place in ocean modeling. Operator splitting of the monotonic van Leer scheme in the vertical direction with MPDATA, QUICKEST, or UTOPIA in the horizontal may be a good solution for biogeochemical ocean modeling where monotonicity, particularly in the vertical, may be required. Alternatively, flux correction could be applied to the QUICKEST or MPDATA schemes; an informed choice would require further investigation.

We have seen that grid stretching is highly effective, and yet it can be, at most, part of the solution for ocean modeling. Regions of highly sheared flow and other problematic features may occur in a much less orderly and convenient sense than in our simple flow field and may even wander throughout the domain, as the Gulf Stream is prone to do.

A set of tracer transport test problems is warranted in order to test advection schemes in three-dimensional primitive equation models. We intend to develop one

Table 5. Maximum Tracer Values Resulting From Advection of an Initially Constant Tracer Field of Value 1.0 After 1 and 10 Time Steps on Regular and Stretched Grids

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Regular n=1</th>
<th>Stretched n=10</th>
<th>Regular n=10</th>
<th>Stretched n=10</th>
</tr>
</thead>
<tbody>
<tr>
<td>CTCS</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>MPDATA</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>UTOPIA</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>QUICKEST</td>
<td>1.0004</td>
<td>1.0009</td>
<td>1.0002</td>
<td>1.0001</td>
</tr>
<tr>
<td>QUICKEST,</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>uncompensated</td>
<td>1.0005</td>
<td>1.0050</td>
<td>1.0002</td>
<td>1.0079</td>
</tr>
<tr>
<td>van Leer [1974]</td>
<td>1.0006</td>
<td>1.0015</td>
<td>1.0003</td>
<td>1.0011</td>
</tr>
<tr>
<td>Donor cell</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
</tbody>
</table>
Figure 10. A zoomed plot of finite difference and reference solutions at four times standard resolution (25 km meridional grid spacing) generated on a stretched grid, using the same stretching function as described in section 4.3. The reference solution is contoured with a solid line. A solution generated with UTOPIA is contoured with a dashed line, which can be seen to depart slightly from the solid line in some places.

or more of these tests in order to test implementations of MPDATA and a QUICKEST-based scheme.

Finally, we suggest that the momentum equations should also be treated with forward-in-time, upwind-weighted integration. We have found that advection through a poorly resolved and highly sheared boundary flow is treated better by forward-in-time, upwind-weighted schemes than by centered-in-space, centered-in-time integration. This finding applies to the advection of either temperature, salt, or mass, though the impact of the resulting errors on the dynamics will be different.

Appendix

Here we consider the convergence of the finite difference and reference solutions in order to validate the accuracy of the numerically obtained reference solution. The finite difference solutions are integrated with UTOPIA on the stretched grid at the standard resolution of 100 zonal grid elements and 63 meridional grid elements and also at doubled resolution (200 x 126) and at four times resolution (400 x 252).

The finite difference solution at four times resolution and the reference solution are shown in Figure 10. The two solutions are nearly indistinguishable in the contour plot. The error measures are recorded in Table 6. In particular, we note that the second moment of the error field $I_2$ drops by approximately a factor of 4 with the first doubling of resolution, as one expects for an $O(\Delta x^2)$ accurate scheme. The $I_2$ error measure drops by a factor of 6 with the second doubling of resolution, and this is again consistent with the expected error scaling of a second-order accurate scheme relative to a reliable reference solution.

Leonard et al. [1994] note that finite difference methods (for which the scalar field represents the nodal point value) and control volume methods (for which the scalar field represents the cell-averaged value) differ above second order. We initialize simulations with nodal values rather than volume averages and do not differentiate carefully between finite difference and control volume methods. We expect we would see a rescaling of error measures if we worked consistently in a control volume formulation but that the hierarchy of error measures would remain unchanged.

Acknowledgments. We thank Piotr Smolarkiewicz for providing a coded version of his MPDATA advection routine and B. P. Leonard for his comments on our manuscript.

References


Leonard, B. P., The ULTIMATE conservative difference

Table 6. Error Measures on Grid for Which $\Delta x$ is Variable, using UTOPIA Scheme at Several Resolutions

<table>
<thead>
<tr>
<th>Resolution</th>
<th>MIN</th>
<th>MAX</th>
<th>$l_1$</th>
<th>$l_2$</th>
<th>$l_{oo}$</th>
<th>V</th>
</tr>
</thead>
<tbody>
<tr>
<td>1x</td>
<td>-0.02152</td>
<td>-0.1077</td>
<td>0.1555</td>
<td>0.1171</td>
<td>0.1112</td>
<td>-0.0810</td>
</tr>
<tr>
<td>2x</td>
<td>-0.00294</td>
<td>-0.0223</td>
<td>0.0337</td>
<td>0.0257</td>
<td>0.0256</td>
<td>-0.0145</td>
</tr>
<tr>
<td>4x</td>
<td>-0.00029</td>
<td>-0.0031</td>
<td>0.0100</td>
<td>0.0043</td>
<td>0.0039</td>
<td>-0.0035</td>
</tr>
</tbody>
</table>

See Table 2 for definitions.

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