Conservative Transport Schemes for Spherical Geodesic Grids: High-Order Flux Operators for ODE-Based Time Integration

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ABSTRACT

Higher-order finite-volume flux operators for transport algorithms used within Runge–Kutta time integration schemes on irregular Voronoi (hexagonal) meshes are proposed and tested. These operators are generalizations of third- and fourth-order operators currently used in atmospheric models employing regular, orthogonal rectangular meshes. Two-dimensional least squares fit polynomials are used to evaluate the higher-order spatial derivatives needed to cancel the leading-order truncation error terms of the standard second-order centered formulation. Positive definite or monotonic behavior is achieved by applying an appropriate limiter during the final Runge–Kutta stage within a given time step.

The third- and fourth-order formulations are evaluated using standard transport tests on the sphere. The new schemes are more accurate and significantly more efficient than the standard second-order scheme and other schemes in the literature examined by the authors. The third-order formulation is equivalent to the fourth-order formulation plus an additional diffusion term that is proportional to the Courant number. An optimal value for the coefficient scaling this diffusion term is chosen based on qualitative evaluation of the test results. Improvements using the higher-order scheme in place of the traditional second-order centered approach are illustrated within 3D unstable baroclinic wave simulations produced using two global non-hydrostatic models employing spherical Voronoi meshes.

1. Introduction

The conservative form of the scalar transport equation within a fluid can be expressed as

$$\frac{\partial (\rho \psi)}{\partial t} = -\nabla \cdot \mathbf{V} \rho \psi,$$

(1)

where $\rho$ is the fluid density, $\psi$ is the mixing ratio, and $\mathbf{V}$ is the fluid velocity. This transport equation appears in all geophysical fluid-flow solvers, and a major portion of a solver’s computational expense in models can arise from its solution for moisture, aerosols, and chemical species. It is generally straightforward to obtain exact conservation of scalar mass in the discrete integration of (1) given its flux form, and exact conservation is highly desirable in many emerging geophysical applications.

Herein, we consider a specific set of spatial discretizations of the flux divergence [the right-hand-side term in (1)], introduced by Hundsdorfer et al. (1995), that can be employed within time-integration schemes using multistage ordinary differential equation (ODE) solvers, such as Runge–Kutta time-integration schemes (see Durran 2010). Furthermore, we introduce extensions of this approach that make use of polynomial reconstructions for use on irregular polyhedral meshes, in our case Voronoi tesselations that are nominally hexagons. We also make use of the finite-volume formalism of these schemes to employ a flux limiter based on Zalesak (1979) to enforce a monotonicity constraint on the solution. We are motivated to further develop these transport schemes because many geophysical fluid-flow solvers use time-integration schemes based on these
ODE solvers, and we want our transport solvers to use the same time-integration schemes and thus be consistent with the flow solver.

In this paper we refer to the scheme order of accuracy based on the accuracy of the spatial discretization of the divergence operator \([\text{the right-hand side of (1)}]\) assuming constant \(\mathbf{V}\) and \(\rho\); that is, we refer to the accuracy of the scalar gradient \(\mathbf{V}\psi\) in the linearized divergence \(\rho\mathbf{V} \cdot \nabla\psi\). In most finite-volume and finite-difference models, the continuity equation \([\text{(1)}\] with \(\psi = 1\) is integrated using second-order-centered spatial discretizations. The resulting mass fluxes \(\rho\mathbf{V}\) are at most second-order accurate, and the overall accuracy and convergence rate of discrete solutions to the transport \([\text{(1)}]\) will be limited to second order. Our past experience (e.g., Wicker and Skamarock 2002) shows that improving the formal accuracy of the scalar gradient discretization significantly improves the accuracy and efficiency of the scalar transport solutions and the atmospheric flow solutions.

A number of transport schemes have been developed for Voronoi (hexagonal) meshes using finite-volume discretizations and single-stage time integration. Lipscomb and Ringler (2005), Yeh (2007), and Miura (2007) develop second-order finite-volume schemes and demonstrate that the schemes are more accurate than the standard second-order-centered spatial discretization of the flux divergence coupled with leapfrog or Runge–Kutta time integration. These schemes use first-order polynomials to reconstruct the scalar distribution. Lashley (2002) and Skamarock and Mutch (2010) have examined extensions to this approach that use second- and fourth-order polynomials in the reconstruction, and they find that the resulting schemes are significantly more accurate than those using the first-order reconstructions. Ji and Xiao (2010) developed a multimoment single-stage solver transport and the shallow-water equations on Voronoi (triangular) meshes and demonstrated third- and fourth-order convergence for variants of their schemes. In contrast to these schemes, we restrict ourselves to scalar transport schemes using multistage ODE solvers. There have been other efforts to use multistage time integration for the transport equation. For example, Weller et al. (2009) developed a shallow-water model using Crank–Nicholson and second-order polynomial reconstruction and demonstrated second-order convergence for the standard shallow-water test cases from Williamson et al. (1992).

We begin in section 2 by motivating and describing the discretization for the irregular mesh. Results from standard transport test cases on the sphere are presented in section 3 and include the standard cosine bell and slotted cylinder translation using a solid-body-rotation flow, the transport of a cosine bell in a deformational flow field, and the transport of Gaussian hills in a deformational flow field. We address scheme efficiency at the end of section 3. In section 4 we present results from 3D baroclinic-wave simulations on the sphere that demonstrate improvements we have observed using our scheme for the thermodynamic variables in adiabatic solvers. We conclude with a summary of our results in section 5.

2. Transport scheme

We define a velocity \(\mathbf{V} = (u, v)\) and density \(\rho\), and we assume that they satisfy a discrete continuity equation consistent with a spatial and temporal discretization of \((1)\). If we assume that the density is constant, we can spatially discretize the rhs term in \((1)\) and cast the transport equation as

\[
\frac{\partial(c)}{\partial t} = L(\mathbf{V}, c),
\]

where the subscripts \(i\) and \(j\) denote values at discrete points in the spatial discretization, and the operator \(L(\mathbf{V}, c) = -\nabla \cdot \mathbf{V}c\) is a discrete form of the divergence operator. We do not lose generality with the constant-density assumption; one can substitute \(\rho\mathbf{V}\) for \(\mathbf{V}\) and multiply the mixing ratio in the time derivative by \(\rho\) in the following discussion to recover \((1)\) as long as a consistent discrete continuity equation is used.

For the temporal integration of \((2)\), we use the Runge–Kutta method described in Wicker and Skamarock (2002) that is referred to as RK3. It is third-order accurate for linear systems and second-order accurate for nonlinear systems (Purser 2007), and it is the basis for the time integration of the Navier–Stokes equations in the Weather Research and Forecasting (WRF) model (Skamarock and Klemp 2008). RK3 uses three stages to advance the solution a single time step \(\Delta t\):

\[
\psi^* = \psi^i + \frac{\Delta t}{3} L(\mathbf{V}, \psi^i),
\]

\[
\psi^{**} = \psi^i + \frac{\Delta t}{2} L(\mathbf{V}, \psi^*),
\]

\[
\psi^{i+\Delta t} = \psi^i + \Delta t L(\mathbf{V}, \psi^{**}).
\]

Other time-integration schemes can be used, for example the time integration schemes described in Durrant (2010), provided that the combination of the spatial and temporal discretizations is stable. The RK3 scheme is stable when combined with many spatial discretizations for transport (see Wicker and Skamarock 2002).

Given the temporal discretization, we turn our attention to the focus of this paper—the spatial discretization of the operator \(L\). On a geodesic mesh such as that depicted in Fig. 1, we can apply the divergence theorem to the right-hand side of \((2)\), resulting in
where $A_i$ is the area of cell $i$, $d_i$ is the length of edge $e_i$, and here $\Delta t$ is the time step of the specific RK3 stage. The instantaneous flux $F_c(\mathbf{V}, \psi) = (\mathbf{V} \cdot \mathbf{n}_i)\psi$, where $\mathbf{n}_i$ is the outward-directed unit normal. Here, the flux divergence involves the summation of fluxes, and (4) has the character of a finite-volume formulation. Equation (4) applies to each Runge–Kutta stage in (3) with the use of the appropriate time step and the evaluation of the flux divergence using the appropriate predictor, and it applies not only to the geodesic mesh but to any cell-based decomposition.

### a. One-dimensional flux calculation

Integration of the transport equation using (3) and (4) requires the specification of the instantaneous flux $F$. There are a number of ways to specify $F$ for models using rectangular orthogonal meshes (e.g., WRF), where the flux computations are performed independently along coordinate directions and result in the sum of the spatially 1D operators. These 1D operators for the flux divergence [the terms multiplied by $\Delta t$ in (4)] can be written as

$$\frac{\partial (u \psi_i)}{\partial x} = \frac{1}{\Delta t} [F_{i+1/2}(u \psi) - F_{i-1/2}(u \psi)] + O(\Delta x^p).$$

The discretization (5) is described as $p - 1$ order accurate because it has a leading error term of order $p$.

The standard second-order operator flux operator is

$$F(u, \psi)_{i+1/2} = u_{i+1/2} \left[ \frac{1}{2} (\psi_{i+1} + \psi_i) \right].$$

The third- and fourth-order flux operators used in WRF can be written as

$$F(u, \psi)_{i+1/2} = u_{i+1/2} \left[ \frac{1}{2} (\psi_{i+1} + \psi_i) - \frac{1}{12} (\delta_x^2 \psi_{i+1} + \delta_x^2 \psi_i) + \text{sign}(u) \frac{\beta}{12} (\delta_x^4 \psi_{i+1} - \delta_x^4 \psi_i) \right],$$

where the coefficient $\beta = 1$ gives the standard formulation for the third-order flux, $\beta = 0$ corresponds to the fourth-order flux (Wicker and Skamarock 2002; Hundsdorfer et al. 1995), the operator $\delta_x^2 \psi_i = \psi_{i+1} - 2 \psi_i + \psi_{i-1}$, and sign($u$) is positive for $u$ indicating flow from cell $i$ to cell $i + 1$. Assuming $\beta = 1$ and $u$ is positive, the third-order flux in (7) can also be written as

$$F(u, \psi)_{i+1/2} = u_{i+1/2} \left[ \frac{1}{2} (\psi_{i+1} + \psi_i) - \frac{1}{6} (\delta_x^2 \psi_i) \right].$$

The upstream nature of the third-order operator is apparent in that the flux in (8) is evaluated using the upwind value of $\delta_x^2 \psi$ in place of the centered evaluation used in the fourth-order scheme [(7) with $\beta = 0$].

The diffusive nature of the third-order operator can be appreciated by computing the flux divergence, which for constant $u$ is given by

$$F(u, \psi)_{i+1/2} - F(u, \psi)_{i-1/2} = u_{i+1/2} \left[ \frac{1}{2} (\psi_{i+1} + \psi_i) - \frac{1}{12} (\delta_x^2 \psi_{i+1} + \delta_x^2 \psi_i) + \frac{\beta}{12} (\delta_x^4 \psi_{i+1} - \delta_x^4 \psi_i) \right] - u_{i-1/2} \left[ \frac{1}{2} (\psi_i + \psi_{i-1}) - \frac{1}{12} (\delta_x^2 \psi_i + \delta_x^2 \psi_{i-1}) + \frac{\beta}{12} (\delta_x^4 \psi_i - \delta_x^4 \psi_{i-1}) \right]
= u_{i+1/2} \left[ \frac{1}{2} (\psi_{i+1} + \psi_i) - \frac{1}{12} (\delta_x^2 \psi_{i+1} + \delta_x^2 \psi_i) \right] - u_{i-1/2} \left[ \frac{1}{2} (\psi_i + \psi_{i-1}) - \frac{1}{12} (\delta_x^2 \psi_i + \delta_x^2 \psi_{i-1}) \right] + u_{i+1/2} \frac{\beta}{12} \delta_x^4 \psi_i.$$
The last term is a fourth-order hyperdiffusion with a hyperviscosity proportional to the Courant number.

Before describing our extension of the flux calculation (7), we would like to point out that the specifications of the scalar value at the cell face [the bracketed terms in (6)–(8)] do not represent different-order interpolations, and their specification is not an interpolation problem. While the bracketed term on the right-hand side of (6) appears as a linear interpolation of the mixing ratio \( \psi \) to the cell face, the bracketed terms in the higher-order fluxes (7) and (8) do not correspond to any higher-order interpolations. The higher-order flux formulations are determined such that the flux divergence in (5) is higher order; that is, the difference of the fluxes should represent a high-order approximation to the gradient of \( \psi \) [the linear operator (5) with constant \( u \)].

### b. Multidimensional flux calculation

The multidimensional flux operator is evaluated by applying the one-dimensional flux operator at each face of a control volume and summing as in (4). In a finite-volume implementation, for two (three) spatial dimensions the flux is multiplied by the length (area) of the cell face where it is evaluated, and this cell-boundary flux integral is divided by the cell area (volume) to complete the spatial-operator approximation for a cell-averaged mixing ratio that can be temporally integrated using (3). The flux operators (6) and (7) can be applied directly in the multidimensional case when the mesh is continuous, that is, for the rectangular meshes used in most mesoscale and global atmospheric models (e.g., Skamarock and Klemp 2008), because the cell values lie along coordinate lines in the global coordinate system describing the mesh. However, the cell values do not lie on global coordinate lines for icosahedral-hexagonal meshes on the sphere; the meshes are irregular and the higher-order operator (7) cannot be directly applied. The second-order operator (6) can be directly used because it employs a simple average of the cell values to the cell face (e.g., Tomita et al. 2001; Walko and Avissar 2008).

We can compute third- or fourth-order-accurate fluxes on irregular Voronoi meshes, similar to (7), by recognizing that the higher-order corrections in (7) are composed of terms approximating second derivatives of the scalar in the direction normal to the edge:

\[
\delta^2_i \psi = \Delta x^2 \frac{\partial^2 \psi}{\partial x^2} + O(\Delta x^4). \tag{10}
\]

In our irregular Voronoi mesh formulation, we replace the operator \( \delta^2_i \psi \) with the second derivative of a polynomial, taken in the direction normal to the cell edge, multiplied by the square of the distance between the cell centers that share that edge. Thus, the general higher-order flux can be written as

\[
F(u, \psi)_{i+1/2} = u_{i+1/2} \left[ \frac{1}{2}(\psi_{i+1} + \psi_i) - \Delta x^2 \frac{\partial^2 \psi}{\partial x^2} \right]_{i+1} + \left( \frac{\partial^2 \psi}{\partial x^2} \right)_{i+1} + \text{sign}(u) \Delta x^2 \beta \left( \frac{\partial^2 \psi}{\partial x^2} \right)_{i+1} - \left( \frac{\partial^2 \psi}{\partial x^2} \right)_{i} \right], \tag{11}
\]

where \( \Delta x \) is the distance between cell centers \( i \) and \( i + 1 \) that share edge \( e \), \( x \) is the direction normal to edge \( e \), and \( u_{i+1/2} \) is the velocity normal to cell edge \( e \) and is positive for flow from cell \( i \) to cell \( i + 1 \).

The formulations (11) and (7) represent third-order \((\beta \neq 0)\) and fourth-order \((\beta = 0)\) accurate algorithms for meshes with constant mesh spacing \( \Delta x \) and constant velocity. For variable mesh spacing, these formulations are no longer third- and fourth-order accurate. Consider the 1D problem with constant velocity \( u = U \) and cell center spacings \( \Delta x_i \) to the left and \( \Delta x_i \) to the right of a given center. If we define the cell center values \( \psi_i \), \( \psi_0 \), and \( \psi_r \), the Taylor series expansion for the second-order-accurate flux divergence (5) and (6) can be written as

\[
\frac{\partial (U \psi)}{\partial x} - U \left[ \frac{\psi_r - \psi_i}{(\Delta x_r + \Delta x_i)} \right] = U \left[ (\Delta x_r - \Delta x_i) \psi_{xx} + \left( \Delta x_i^2 + \Delta x_r^2 \right) \psi_{xxx} \right] \frac{1}{12(\Delta x_r + \Delta x_i)} - \frac{(\Delta x_i^4 - \Delta x_r^4)}{24(\Delta x_r + \Delta x_i)} \psi_{xxxx} + O(\Delta x^4),
\]

The nominally second-order scheme is only first-order accurate for a nonuniform mesh spacing, but for constant mesh spacing \( \Delta x_r = \Delta x_i \) the truncation error terms multiplied by the second and fourth derivatives drop out and the leading-order truncation error is proportional to \( \Delta x^2 \). The higher-order approximations (11) and (7) result in the cancellation of the term multiplied by the third derivative when \( \Delta x_r = \Delta x_i \), and the third-order scheme introduces a fourth-order damping term, as given in (9). For nonuniform mesh spacing, the leading-order truncation error term for the nominally fourth-order scheme is \( (\Delta x_r - \Delta x_i) \psi_{xx}/6 \). Thus, the scheme is formally only first-order accurate, but with a leading-order truncation error term much smaller than that for the second-order scheme. Interestingly, the term containing the third-order derivative does cancel in the variable-mesh higher-order formulation.
The polynomials from which the second derivatives used in (11) are computed are determined using least squares fits to the cell-average values of $\psi$. For example, consider the computation of the flux for cell edge $e_1$ in Fig. 1. Cell edge $e_1$ is shared by cells $C_0$ and $C_1$, and second derivatives in the $C_0C_1$ direction are needed at points $C_0$ and $C_1$ to compute the flux (11). Second-order polynomials are used in the least squares fit,

$$\psi = c_0 + c_x x + c_y y + c_{xx} x^2 + c_{xy} xy + c_{yy} y^2,$$

and we use the cell-center values and the values of the neighboring cells (those that share an edge with that cell) for computing the least squares fit polynomial. Thus, in Fig. 1 values from cells 0–6 are used to compute the polynomial for cell 0, and values from cells 0–2 and 6–9 are used to compute the polynomial for cell 1.

Defining the cell-averaged scalar mixing ratio values used in the least squares fit for a cell as $s = [\psi_{0}, \ldots, \psi_{m}]^T$ with dimension $m$, the polynomial coefficients $f = [c_0, \ldots, c_y]^T$ of dimension $n = 6$, and the polynomial matrix $P = (1, x, y, x^2, xy, y^2)$, we compute the least squares fit polynomial following Strang (1980):

$$f = (P^T P)^{-1} P^T s = Bs,$$

where $B$ is an $(n \times m)$ matrix. From $B$, we need only the weights with which to multiply $s$ to compute the second derivative in the $C_0C_1$ direction. In practice the weights are computed and stored before the integration. Specifically, we store two sets of weights for each edge corresponding to those needed to compute the normal second derivative in each of the two adjoining cells. Thus, during the integration the second derivative computations are simple vector–vector multiplies.

We use spherical centroidal Voronoi tesselations for computations on the sphere. The cell centers are located at the cell center of mass on these meshes, and the great-circle arcs connecting cell centers intersect the cell edges at right angles. Further information concerning these meshes can be found in Ringler et al. (2008, 2010). Following Skamarock and Menchaca (2010), we define a 2D $(x, y)$ tangent plane touching the sphere at the center of the cell for use in computing the least squares fit polynomial (12) for that cell, as depicted in Fig. 2. The neighboring points used in the calculations are projected onto the plane using the great-circle distances between the cell-center point and the neighbor points and using the angles at the cell-center point defined by the great-circle arcs between these points and the cell-center point. This procedure preserves the distance between the tangent (center) point and outlying points and their direction relative to the tangent point in the tangent plane approximation.

Other projections are possible, such as a projection perpendicular to the tangent plane, or perpendicular to the sphere (these alternatives are depicted in Fig. 2). Our experiments indicate that the results are insensitive to the details of the tangent-plane approximation.

The transport schemes described by (3), (6), and (11) are not monotonic. We use the flux-corrected transport (FCT) limiter of Zalesak (1979) to recover positive definiteness or monotonicity when desired. The limiter is applied on the last step of the Runge–Kutta solver, as described in Wang et al. (2009). FCT renormalization requires first updating the field using a first-order upwind flux. Our higher-order corrective fluxes are the full fluxes minus the upwind fluxes, which are then renormalized to achieve positive definiteness or monotonicity, and these renormalized fluxes are used to complete the update.

3. 2D test results

In the following section we present test results for 2D scalar transport on the sphere using our schemes. The cosine bell test case from Williamson et al. (1992) is widely used and cited in the literature, as is the slotted cylinder test case, thus allowing direct comparison with
other schemes. The deformational flow test case is similar to that presented in Blossey and Durran (2008) and represents a more demanding test because the flow is deformational. The test case using Gaussian hills allows us to demonstrate the formal accuracy (convergence rate) of our scheme because the scalar distribution is infinitely differentiable, whereas second and higher derivatives of the cosine bell are discontinuous.

a. Cosine bell

The advection of a cosine bell test is described in Williamson et al. (1992), where the flow field representing solid-body rotation transports the bell once around the sphere and returns it to its initial location without any distortion during the transport. Following Williamson et al. (1992), the bell is defined as

$$\psi = \begin{cases} (\psi_0/2)[1 + \cos(\pi r/R)] & \text{if } r < R, \\ 0 & \text{if } r \geq R, \end{cases}$$

where $\psi_0 = 1000$, the bell radius $R = a/3$, and $a$ is the radius of the sphere. The equatorial velocity $u_0 = 2\pi a/(12 \text{ days})$ (relative to the equator of the solid-body rotation). Integration parameters for these simulations are given in Table 1.

Figure 3 presents results for this test case using the second-, third-, and fourth-order schemes with and without the monotonic limiter. The results clearly show the large phase errors associated with the shorter wavelengths for the second-order scheme. The third- and fourth-order schemes have dramatically reduced phase errors relative to the second-order scheme. The third-order scheme uses $\beta = 1$ in (11) for these tests, and the results

<table>
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<th>Cells</th>
<th>Avg $\Delta x_e$</th>
<th>Cosine bell $\Delta t$ (s)</th>
<th>Deformational flow $\Delta t$ (s)</th>
<th>Gaussian hills $\Delta t$ (s)</th>
</tr>
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Fig. 3. Cosine bell after one revolution on the sphere. The contour interval is 100 and the thick contours show the exact solution for $\psi = 100$ and 800. The simulations were performed on the 10 242-cell mesh.
show significant damping for the third-order scheme in comparison with the fourth-order scheme. All three schemes produce values less than zero when the monotonic limiter is not used. Additional damping is evident when the monotonic limiter is used in the second- and fourth-order results, as seen in the reduction in the peak values of the bell. The third-order scheme does not show any significant reduction in amplitude when the limiter is used, but this scheme already has significant damping in its formulation. Also apparent in the monotonic fourth-order scheme results is a significant asymmetry in the solution when the limiter is used. This asymmetry is not apparent in the results from the third-order scheme.

The $L_2$ error norms, 
\[
L_2 = \left[ \sum_{\text{cells}} A_{\text{cell}} (\psi_{\text{cell}} - \psi_{\text{exact}})^2 \right]^{1/2} / \left( \sum_{\text{cells}} A_{\text{cell}} \psi_{\text{exact}}^2 \right)^{1/2},
\]
are presented for this test case in Fig. 4. The error norms confirm the qualitative results in Fig. 3 that the third- and fourth-order schemes produce more accurate solutions than the second-order scheme. The second-order scheme shows slightly less than second-order convergence with and without the limiter. The fourth-order scheme shows slightly less than second-order convergence without the limiter and slightly greater than second-order convergence with the limiter, while the third-order scheme has slightly greater than second-order convergence for the unlimited scheme and approaches third-order convergence for the limited scheme. The solution error is reduced for the second- and third-order schemes comparing the limited to the unlimited schemes, but the solution error increases when using the limiter with the fourth-order scheme, probably due to the appearance of the asymmetry that arises from the interaction of the fourth-order scheme and the limiter. The higher-than-second-order convergence rate observed for the third-order scheme using the limiter is consistent with the results from upwind-biased schemes given in Skamarock and Menchaca (2010) and Miura (2007) for this test case. As is noted in Skamarock and Menchaca (2010), this result did not extend to the more demanding test cases that use a time-dependent deformational flow that better characterizes atmospheric flows, and next we test these schemes using such a flow.

b. Blossey and Durran deformational flow test

We use a 2D deformational flow test case presented in Blossey and Durran (2008) that has been extended to the sphere by Skamarock and Menchaca (2010). The test case is depicted in Fig. 5 and is taken from Skamarock and Menchaca. A background solid-body-rotation flow advects the cosine bell in a clockwise direction about the pole, and the cosine bell is deformed by an additional time-dependent deformational flow component given by
\[
\Psi(r, t) = \frac{4\pi a^2}{T} \left\{ \sin \lambda \cos \left( \frac{2\pi}{T} \right) \frac{r^2}{2} + \frac{1}{96} \log(1 - 16r^2 + 256r^4) - \frac{1}{48} \log(1 + 16r^2) - \frac{\sqrt{3}}{48} \arctan \left( \frac{1 - 32r^2}{\sqrt{3}} \right) \right\},
\]
and with the limiter is used. The third-order scheme already has significant damping in its formulation. Also apparent in the deformational fourth-order scheme results is a significant asymmetry in the solution when the limiter is used. This asymmetry is not apparent in the results from the third-order scheme.

The $L_2$ error norms, 
\[
L_2 = \left[ \sum_{\text{cells}} A_{\text{cell}} (\psi_{\text{cell}} - \psi_{\text{exact}})^2 \right]^{1/2} / \left( \sum_{\text{cells}} A_{\text{cell}} \psi_{\text{exact}}^2 \right)^{1/2},
\]
where \( \tilde{r} = \phi / \pi \) and the positive (negative) sign is used in the Northern (Southern) Hemisphere. The streamfunction is defined at the cell vertices and the cell-edge velocity is computed by taking the difference between the streamfunction values at the vertices of the edge divided by the great-circle distance between these vertices. The streamfunction is discontinuous and multivalued at the equator, so discrete differentiation for edges crossing the equator is accomplished by adding the differences on both sides of the equator taking into account the sign change in (15).

Results computed on the 40 962-cell mesh are presented in Fig. 6 for the second-, third-, and fourth-order schemes both with and without the limiter, and parameters for these simulations are given in Table 1. The third- and fourth-order schemes are much more accurate than the second-order scheme. Significant asymmetries are introduced when using the monotonic limiter with the fourth-order scheme, and solution amplitude is reduced when the monotonic limiter is used with the second- and fourth-order schemes whereas there is no significant reduction in amplitude for the third-order scheme when using the limiter. The \( L_2 \) error norms are plotted in Fig. 7, and reveal that the schemes retain their approximately second-order convergence and that the convergence rates are reduced when the limiter is used for the second- and fourth-order schemes. Also, the third-order scheme has somewhat greater than second-order convergence when the monotonic limiter is used, and the convergence rate is enhanced, and errors are lowered, when the limiter is used. Again, the asymmetries introduced when the monotonic limiter is used with the fourth-order scheme accompany the greater solution error.

c. Extension of the third-order scheme

The standard third-order scheme from Hundsdorfer et al. (1995) and Wicker and Skamarock (2002) has the parameter \( \beta = 1 \) in (11). The resulting fourth-order hyperdiffusion given in (9) provides the damping that is apparent in the third-order results. The fourth-order scheme, recovered by setting \( \beta = 0 \), exhibits pronounced asymmetries and generally nonsmooth solutions when used with the FCT-based monotonic limiter (e.g., Figs. 3 and 6).

We would like to maintain solution symmetries and smoothness in addition to monotonicity, while minimizing damping, for our higher-order scheme. Toward this end, we have experimented with the parameter \( \beta \), using \( 0 \leq \beta \leq 1 \) in (11). A plot showing the results of the deformational flow test case is given in Fig. 8 where solutions with \( \beta = 1, 0.5, 0.25, \) and \( 0 \) are plotted; the fourth-order result (\( \beta = 0 \)) is reproduced from Fig. 7 for convenience, and the nonsmooth trailing edge (the right side of the cosine bell) is obvious. The decreased damping resulting from decreasing \( \beta \) is easily observed in these solutions. Very little asymmetry is apparent in the solutions using nonzero values for \( \beta \), and there is no obvious solution degradation at the trailing edge of the bell, even when using \( \beta = 0.25 \). Figure 9 shows the \( L_2 \) error norms for the deformational flow test case using the four values of \( \beta \) for which the solutions were plotted in Fig. 8. The \( L_2 \) errors using \( \beta = 0.25 \) are equivalent to or lower than those for the fourth-order scheme (\( \beta = 0 \)), and show better than second-order convergence compared to the second-order convergence produced by the fourth-order scheme.

Both the \( L_2 \) error norms given in Fig. 9 and the qualitative plots of the solution fields given in Fig. 8 strongly suggest that, for smooth scalar fields, the flux equation

![Fig. 5. Exact solution for the Blossey and Durran (deformational flow) test case adapted to the sphere, from Skamarock and Menchaca (2010).](image-url)
be used with $\beta = 0.25$ when monotonic limiting is desired. When the limiter is not used, the third-order scheme with $\beta = 0.25$ and the fourth-order scheme produce very similar results, and the $L_2$ error norms for the third-order scheme are just slightly higher than those for the fourth-order scheme.

d. Gaussian hills

This test case uses the deformational nondivergent flow described in section 3.2.1, case 1, in Nair and Lauritzen (2010), on which a solid-body-rotation flow has been superposed. The initial scalar distribution is composed of a superposed pair of Gaussian hills as given in Nair and Lauritzen’s Eq. (14) with centers located on the equator at $\pm \pi/6$ radians longitude. This scalar distribution is continuously differentiable; hence, the convergence rate of the solution error will indicate the order of accuracy of the transport scheme.

In this test case the scalar is transported once around the sphere. The solutions at times $t = 0, t = T/2,$ and $t = T$ are given in Fig. 10. During the first half rotation, the flow is distorted by the deformational flow, and during the second half rotation the deformational flow is reversed such that the initial and final scalar distributions are identical in the exact solution.

Figure 11 shows the error norms for this test case using the third-order scheme using $\beta = 0.25$ both with and without the monotonic limiter. We compute the $L_2$ error norm as indicated earlier, and the $L_1$ and $L_{\infty}$ error norms are computed as

$$L_1 = \sum_{\text{cells}} A_{\text{cell}} \frac{\text{abs}(\psi_{\text{cell}} - \psi_{\text{exact}})}{\sum_{\text{cells}} A_{\text{cell}} \text{abs}(\psi_{\text{exact}})}$$

and

$$L_{\infty} = \max \{\text{abs}(\psi_{\text{cell}} - \psi_{\text{exact}})\}.$$

The $L_1$, $L_2$, and $L_{\infty}$ error norms indicate that the unlimited scheme is third-order accurate. We infer from these results that third-order accuracy can be expected...
as long as the mesh is sufficiently smooth, as is the case here with our quasi-uniform Voronoi mesh. The limited scheme shows something less than third-order convergence in all three norms, as expected, and the $L_\infty$ and $L_2$ norms show the most significant degradation in convergence relative to the unlimited scheme.

e. Slotted cylinder

The slotted-cylinder test is identical to the cosine-bell test except that a cylinder replaces the cosine bell. We use the initial cylinder from Lipscomb and Ringler (2005) that has a radius $R = a/2$, slot width of $a/6$, and slot length of $5a/6$; the edges of the cylinder are discontinuous. Results for this test case are given in Fig. 12, where the cylinder is translated once around the equator of the sphere. The monotonic limiter produces a solution that is appropriately bounded between its initial range $0 \leq \psi \leq 1000$ for all the schemes, and the cylinder should be symmetric about the line passing through the central axis of the slot. The phase errors inherent in the second-order scheme result in significant distortion of the cylinder, particularly at the trailing edge of the cylinder, consistent with the results from the cosine bell and deformational flow test cases. Much smaller asymmetries are apparent in the third- and fourth-order results. The fourth-order results are much less smooth, and somewhat more asymmetric, than the third-order results. Based on these results, we recommend that the third-order scheme with $\beta = 0.25$ be used in all applications using the monotonic limiter.

f. Efficiency

In addition to scheme accuracy as a function of mesh density, the computational cost of a scheme must be considered in order to assess the overall scheme efficiency. One approach to evaluating scheme efficiency is to examine error as a function of cost rather than as a function of mesh density. It is, however, difficult to meaningfully quantify cost given the different approaches to coding, different compilers, and different computer architectures that can affect simulation cost. We have run our code on a single-processor computer and isolated the time taken in the transport calculations, and we have found that the transport costs scale consistently for the tests we have performed in this paper. Relative to the second-order scheme with no limiter, we find that the second-order scheme with the limiter has a cost factor of approximately 1.3 (i.e., the second-order scheme with the limiter takes 1.3 times the wall-clock
time to complete the transport calculations relative to the second-order scheme without the limiter). The third-order scheme without (with) the limiter has a cost factor of 1.7 (2.0), and the fourth-order scheme has a cost factor of 1.6 (1.9). The $L_2$ error norms plotted as a function of normalized cost for the deformational flow test case are given in Fig. 13, in this case including results for both the limited and unlimited third-order scheme using $\beta = 0.25$ in (11). In all cases the third- and fourth-order schemes are much more efficient than the second-order scheme. For the unlimited transport, the fourth-order scheme is slightly more efficient than the third-order scheme except at the coarsest resolution. Conversely, the limited third-order scheme is slightly more efficient than the limited fourth-order scheme except at the coarsest resolution. There is very little difference in the $L_2$ errors, and cost, between the third- and fourth-order schemes. Based on the $L_2$ error norms, and on the qualitative scalar-field plots presented in Figs. 3, 6, 8, and 12, we recommend either the third-order scheme with $\beta = 0.25$ or the fourth-order scheme for applications where a monotonic limiter is not needed, and the third-order scheme with $\beta = 0.25$ in (11) for use with the monotonic limiter.

4. 3D test results

We have tested these transport schemes in the non-hydrostatic atmospheric solvers within the Icosahedral Nonhydrostatic (ICON; Gassmann 2010; Rıpodos et al. 2009; Gassmann and Herzog 2008) model and the Model for Prediction Across Scales (MPAS; Skamarock et al. 2010). These models both use spherical Voronoi horizontal meshes and a C-grid staggering of the prognostic variables. The transport algorithms are applied only to the

FIG. 9. The $L_2$ error norms for the deformational flow test case at time $T/2$ using (11) with different values of the filter parameter $\beta$. The monotonic limiter is used to produce these results.

FIG. 10. Scalar distribution for the Gaussian hills test case at times $t = 0$, $T/2$, and $T$.

FIG. 11. Error norms for the Gaussian hills test case at time $t = T$ using (19) with $\beta = 0.25$. Both limited and unlimited results are shown. The unlimited scheme is exhibiting third-order convergence (dashed lines) while the limited scheme is converging at less than third order (solid lines).
transport of potential temperature in the full model; the remaining numerics employ second-order-accurate spatial discretizations.

The test case we have used is the unstable baroclinic wave test described in Jablonowski and Williamson (2006). In this test, unstable zonally symmetric jets exist in the Northern and Southern Hemispheres and an initial perturbation in the zonal velocity initiates a baroclinic wave train. No analytic solution exists for this test and high-resolution solutions are used as reference solutions for computing error norms. We have configured the ICON and MPAS models as described in Jablonowski and Williamson (2006). Frontal collapse and wave breaking begin to occur by day 9, and the solutions at earlier times appear to converge based upon visual inspection at the horizontal resolution of the 163 842-cell mesh (i.e., about \( \frac{1}{2}^\circ \) at the equator).

In the Jablonowski and Williamson tests, the only model tested that did not use a latitude–longitude mesh was the GME model (Majewski et al. 2002) developed and used by the German Weather Service (Deutscher Wetterdienst, DWD). At coarse resolutions the GME model showed significantly greater phase errors compared to the other models. The phase error is defined as the longitudinal phase shift needed to minimize the \( L_2 \) error norm for the surface pressure field. Figure 14 shows the phase errors for the GME model test reported in Jablonowski and Williamson and for configurations of the ICON model and the MPAS model using second- and third-order (\( \beta = 0.25 \)) transport schemes described in this paper. The 10 242-cell mesh is used in these tests and the wave train is adequately resolved at this mesh density. For the second-order transport schemes (including the GME configuration), the error growth is similar for all...
three models but the ICON and MPAS models have a lower phase error at any given time. We speculate that this may reflect the difference between the A-grid staggering used in the GME model and the C-grid staggering used in both ICON and MPAS, but we have no other evidence with which to evaluate this speculation at this time. Both the ICON and MPAS models show significant reductions in the phase errors using the third-order transport scheme, where both the absolute errors and their growth rate are reduced. The fourth-order scheme possesses phase errors similar to the third-order scheme as expected from theory.

5. Summary

We have proposed higher-order flux-operator formulations for transport algorithms used within Runge–Kutta time-integration schemes on irregular icosahedral (hexagonal) meshes. One-dimensional flux operators are currently used on regular orthogonal meshes in a number of atmospheric models (e.g., WRF; Skamarock and Klemp 2008). The multidimensional implementations involve evaluating the fluxes in each coordinate direction on each cell face, summation of these 1D fluxes, and time integration using some appropriate scheme (e.g., Runge–Kutta, leapfrog, etc.). The greater-than-second-order-accurate 1D operators are not valid approximations on irregular meshes, and we use 2D least squares fit polynomials for the transported scalars to evaluate alternative forms of these higher-order flux operators. On the spherical centroidal Voronoi tessellation (SCVT) meshes, major improvements in accuracy and efficiency are realized by using the generalized third- and fourth-order fluxes. The use of a flux limiter to achieve monotonicity results in significant unphysical asymmetries developing in the test case solutions when using the fourth-order flux scheme. We have found that we can obtain solutions that are more accurate than those found when using the flux-limited fourth-order scheme by employing the flux-limited third-order scheme with a hyperviscosity of one-quarter the value used in the usual formulation \( \beta = 0.25 \) in (11) as opposed to \( \beta = 1 \).

The third- and fourth-order formulations are evaluated using standard transport tests on the sphere, including the transport of a cosine bell and slotted cylinder by solid-body-rotation flow, a deformational flow test case of Skamarock and Menchaca (2010) that extends the 2D planar test of Blossey and Durran (2008), and a deformational flow test case using a Gaussian hill scalar distribution modified from Nair and Lauritzen (2010).

The Gaussian hills test case demonstrates that the scheme is third-order accurate when using a smooth velocity field. The third- and fourth-order schemes are significantly more efficient than the standard second-order scheme based on results from the deformational flow test case of Skamarock and Menchaca (2010), and the scheme is more accurate than other schemes for the Voronoi and icosahedral (hexagonal) meshes in the literature we have examined. Finally, the beneficial effects of using the higher-order scheme in place of the traditional
second-order centered approach is illustrated in 3D unstable baroclinic wave simulations using two global non-hydrostatic models currently under development: the MPAS model and a hexagonal mesh formulation of the ICON model. In both of these models the higher-order transport operators, used for transport of the potential temperature in the dry simulations, reduce the phase errors in the baroclinic waves by slightly less than a factor of 2 compared to the second-order scheme and slightly less than a factor of 3 compared to the GME model results reported in Jablonowski and Williamson (2006). The results also show that the MPAS and ICON models produce lower phase errors than the GME model even when using the second-order scheme, perhaps indicating a difference between the unstaggered A-grid formulation in the GME model and the C-grid formulations in the MPAS and ICON models.

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