A comparison of variational upwinding schemes for geophysical fluids, and their application to potential enstrophy conserving discretisations

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Abstract

Methods for stabilising the turbulent cascade of potential enstrophy are analysed and compared for a compatible finite element discretisation of the rotating shallow water equations. These different approaches to upwinding the potential vorticity include the well-known anticipated potential vorticity method (APVM), streamwise upwind Petrov-Galerkin (SUPG) method, and a more recent method where the trial functions are evaluated downstream within the reference element. In all cases the upwinding scheme conserves both potential vorticity and energy, since the antisymmetric structure of the equations is preserved. The APVM leads to a symmetric definite correction to the potential enstrophy that is dissipative and inconsistent. The SUPG scheme introduces a consistent correction to the APVM scheme that acts as a backscatter term ensuring a richer depiction of turbulent dynamics. The downwinded trial function formulation results in the advection of downwind corrections, which analysis and numerical experiments show to be quantitatively similar to the SUPG scheme for a turbulent shear flow. The main difference between the SUPG and downwinded trial function schemes is in the energy conservation and residual errors. If just two nonlinear iterations are applied then the energy conservation errors are improved for the downwinded trial function formulation, reflecting a smaller residual error than for the SUPG scheme.

We also present new temporal formulations by which potential enstrophy is exactly integrated across each time level. Results using these formulations are observed to be stable in the absence of any dissipation, despite the aliasing of grid scale turbulence. Using such a formulation and the APVM with a coefficient \(O(100)\) times smaller that its regular value leads to turbulent spectra that are greatly improved at the grid scale over the SUPG and downwinded trial function formulations with unstable potential enstrophy errors.

1. Introduction

Two dimensional turbulence in geophysical fluids involves a nonlinear cascade of energy to large scales and of potential enstrophy to small scales. Consequently such flows may be stabilised via the removal of potential enstrophy at small scales, via the upwinding of the potential vorticity, without breaking energy conservation. This may be achieved by replacing the potential vorticity in the vector invariant form of the momentum equation with a value sampled at some upstream location, as is the case for the well-known anticipated potential vorticity method (APVM) [1], or alternatively via a variational approach by which the test functions are weighted towards an upstream location, such as the streamwise upwind Petrov-Galerkin (SUPG) [2] or variational multiscale method (VMS) [3]. Both the APVM [4] and SUPG [5] methods have previously been used in finite element models of geophysical systems for the energetically consistent transport of material quantities (vorticity [5], potential vorticity [6,7] and potential temperature [8]). A similar approach has also been applied in a finite volume scheme for the shallow water equations derived from a variational principle [9], and VMS approaches have been applied to spectral element discretisations of the compressible Euler equations for atmospheric dynamics [10].

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In the present study the APVM and SUPG methods are compared to a more recent approach by which the potential vorticity trial functions are evaluated at downstream locations within the reference element \[11\] in terms of their consistency, conservation properties and residual errors. This reference element stabilisation has been used previously for the stabilisation of both the potential enstrophy for the shallow water equations, in which case it is applied by downwinding the trial functions \[11\], and to the potential temperature in the 3D compressible Euler equations, in which case it is applied as the upwinding of the test functions \[12\]. In the context of strong form differential operators, for which the differential operator is applied to the trial function (such as the divergence of a mass flux in \(H(\text{div}, \Omega)\) for the flux form advection of some quantity in \(L^2(\Omega)\)), this is achieved via the upwinding of the test function (provided that the test function is \(C^0\) continuous across element boundaries in the direction of the flow). For a weak form differential operator however (such as material advection as the adjoint of the aforementioned flux form operator) this reference element upwinding is conversely applied via the downwinding of the trial functions \[11\].

The principal contributions of this paper are the comparison of the recently developed downwinded trial function method of potential enstrophy stabilisation to the well established APVM and SUPG methods, both in terms of analysis and numerical experiments. We also introduce a new method of exactly integrating the potential enstrophy across each time level. For an implicit time integrator this new temporal representation of the potential enstrophy allows for the simulation of well developed turbulence on the sphere without any form of dissipation whatsoever, since the turbulent cascade of potential enstrophy to the grid scale is well controlled.

The remainder of this article proceeds as follows: In Section 2, the mixed finite element discretisation of the rotating shallow water equations and its conservation properties are introduced. The APVM, SUPG and downwinded trial function formulations of the potential enstrophy are analysed in the context of this discretisation in Section 3. Section 3 also introduces new time discretisations for the potential vorticity at first and second order, which allow for the exact integration of the potential enstrophy across the time level, such that simulations may be run to a mature turbulent state without any form of dissipation whatsoever. Results comparing the three upwinding schemes for the solution of a shear flow instability test case \[13\] are presented in Section 4, and conclusions are discussed in Section 5.

2. Mixed finite element discretisation the rotating shallow water equations

The rotating shallow water equations for the evolution of the velocity, \(u\) and depth, \(h\), within a two dimensional domain \(\Omega \subset \mathbb{R}^2\) may be expressed as

\[
\begin{align*}
\frac{\partial u}{\partial t} + qF^\perp + \nabla P &= 0, \\
\frac{\partial h}{\partial t} + \nabla \cdot F &= 0,
\end{align*}
\]

(1a)

(1b)

where

\[
F = hu,
\]

(2a)

\[
P = \frac{1}{2}u \cdot u + gh,
\]

(2b)

\[
q = \frac{\nabla \times u + f}{h},
\]

(3)

is the potential vorticity, while \(f\) is the Coriolis term. The operator \(\perp\) denotes rotation as \(F^\perp = [-F \cdot \hat{y}, F \cdot \hat{x}]\) for the unit vectors \([\hat{x}, \hat{y}]\) which specify a coordinate system for \(\Omega\). We further note that both \(q\) and \(f\) are scalar quantities within \(\Omega\), however for the extension to a three dimensional domain these may be regarded as the radial components of a vector quantity.

In order to spatially discretise the above system we introduce finite dimensional subspaces \(\mathcal{V}_0 \subset H^1(\Omega)\), \(\mathcal{V}_1 \subset H(\text{div}, \Omega)\), \(\mathcal{V}_2 \subset L^2(\Omega)\), which may be compatibly mapped to one another via the discrete De-Rham complex of the form \[2, 14, 15\]

\[
\mathbb{R}^2 \longrightarrow \mathcal{V}_0 \longrightarrow \mathcal{V}_1 \longrightarrow \mathcal{V}_2 \longrightarrow 0.
\]

(4)
The prognostic equations (1) are then solved for the discrete approximations \( q_h \in \mathcal{V}_0, \ u_h, F_h \in \mathcal{V}_1, \ h_h, P_h \in \mathcal{V}_2 \) by multiplying by the test functions \( v_h, \phi_h \in \mathcal{V}_2 \) respectively. We emphasise the difference here between trial functions, basis functions used to represent the solution fields, \( q_h, u_h, F_h, h_h, P_h \), and test functions, \( v_h, \phi_h \), basis functions against which the discrete form of the differential equations are weighted in order to derive a variational form of the system. Integrating over the domain \( \Omega \) using integrating by parts and assuming periodic boundary conditions, the spatially discrete form of the equations are given as

\[
\int v_h \frac{\partial u_h}{\partial t} d\Omega + \int v_h q_h F^2_h d\Omega - \int \nabla \cdot v_h P_h d\Omega = 0 \quad \forall v_h \in \mathcal{V}_1, \tag{5a}
\]

\[
\int \phi_h \frac{\partial h_h}{\partial t} d\Omega + \int \phi_h \nabla \cdot F_h d\Omega = 0 \quad \forall \phi_h \in \mathcal{V}_2. \tag{5b}
\]

The discrete form of the energy is given as

\[
\mathcal{H}_h(u_h, h_h) = \int \frac{1}{2} h_h u_h \cdot u_h + \frac{1}{2} g h_h^2 d\Omega. \tag{6}
\]

The variational derivatives of the energy with respect to the solution variables, \( u_h, h_h \) may be computed discretely as the perturbation of the solution variables in some arbitrary test direction \( v_h, \phi_h \) by some small value \( \epsilon \) in the limit that \( \epsilon \to 0 \) \( \mathcal{O} \). The corresponding mass flux and Bernoulli potential are therefore given in analogy to (2) as

\[
\frac{d}{d\epsilon} \mathcal{H}_h(u_h + \epsilon v_h, h_h) \big|_{\epsilon=0} = \int v_h \cdot \frac{\partial \mathcal{H}_h}{\partial u_h} d\Omega = \int v_h \cdot F_h d\Omega = \int v_h \cdot u_h d\Omega d\Omega \quad \forall v_h \in \mathcal{V}_1, \tag{7a}
\]

\[
\frac{d}{d\epsilon} \mathcal{H}_h(u_h, h_h + \epsilon \phi_h) \big|_{\epsilon=0} = \int \phi_h \frac{\partial \mathcal{H}_h}{\partial h_h} d\Omega = \int \phi_h P_h d\Omega = \int \phi_h \frac{1}{2} u_h \cdot u_h + g h_h^2 d\Omega \quad \forall \phi_h \in \mathcal{V}_2. \tag{7b}
\]

Moreover, the discrete form of the potential vorticity, \( q_h \in \mathcal{V}_0 \) is determined in analogy to (5) as

\[
\int \psi_h h_h q_h d\Omega = \int -\nabla \cdot \psi_h \cdot u_h + \psi_h f_h d\Omega \quad \forall \psi_h \in \mathcal{V}_0, \tag{8}
\]

with \( f_h \in \mathcal{V}_0 \) being the discrete representation of the Coriolis term.

### 2.1. Conservation properties

In order to describe the semi-implicit solution of the rotating shallow water equations, we first introduce the dual spaces \( \mathcal{V}^*_0, \mathcal{V}^*_1, \mathcal{V}^*_2 \) and the \( L^2(\Omega) \) inner product as \( (a, b) = \int a b d\Omega \). The duality pairing is given as \( (a, \cdot) \), which maps coefficients of \( a \) to coefficients in the corresponding dual space. The linear mass matrices are then given as \( \mathbf{M}_1 : \mathcal{V}_1 \rightarrow \mathcal{V}^*_1 \) for which \( \mathbf{M}_1 v_h := (v_h, \cdot), \forall v_h \in \mathcal{V}_1 \) and \( \mathbf{M}_2 : \mathcal{V}_2 \rightarrow \mathcal{V}^*_2 \) for which \( \mathbf{M}_2 \phi_h := (\phi_h, \cdot), \forall \phi_h \in \mathcal{V}_2 \). We also introduce the divergence operator, \( \mathbf{D} : \mathcal{V}_1 \rightarrow \mathcal{V}^*_1 \) as \( \mathbf{D} v_h := \langle \nabla \cdot v_h, \cdot \rangle \) and the rotational operator \( \mathbf{C} : \mathcal{V}_0 \times \mathcal{V}_1 \rightarrow \mathcal{V}^*_1 \) as \( \mathbf{C}(\phi_h, v_h) := \langle \phi_h v_h^\top, \cdot \rangle \).

The energy conserving structure of the spatially and temporally discrete formulation of the rotating shallow water equations (5) and (7) is exposed by expressing these in skew-symmetric form as:

\[
\left[ \begin{array}{c}
\mathbf{M}_1 \left( u_h^{n+1} - u_h^n \right) \\
\mathbf{M}_2 \left( h_h^{n+1} - h_h^n \right)
\end{array} \right] + \Delta t \left[ \begin{array}{c}
\mathbf{C} (\cdot, \bar{q}_h) \\
\mathbf{D}
\end{array} \right] \begin{bmatrix} F_h \\ P_h \end{bmatrix} = 0 \tag{9}
\]

where \( F_h, P_h \) are the exact time integrals of the mass flux and Bernoulli potential respectively. Since we compute solutions only at the beginning and end of the time level using our implicit time integrator, and not at intermediate times, we can only assume solutions that are piecewise linear in time. These piecewise linear representations of the variational derivatives can be integrated exactly between time levels \( n \) and \( n + 1 \) using Simpson’s rule, resulting in implicit expressions for the exact second order temporal integrals of the variational derivatives (7) as (7)[17][18]

\[
\int v_h \cdot \overline{F}_h d\Omega = \frac{1}{6} \int v_h \cdot u_h^{n+1} + v_h \cdot u_h^n + v_h \cdot u_h^n (h_h^{n+1} + 2 h_h^n) d\Omega \quad \forall v_h \in \mathcal{V}_1, \tag{10a}
\]

\[
\int \phi_h \overline{P}_h d\Omega = \frac{1}{6} \int \phi_h (u_h^{n+1} + u_h^n + u_h^n) d\Omega + \frac{g}{2} \int \phi_h (h_h^{n+1} + h_h^n) d\Omega \quad \forall \phi_h \in \mathcal{V}_2. \tag{10b}
\]
Note that the variational derivatives are continuous both within and between time levels, since $u_h^{n+1}, h_h^{n+1}$ at the end of a given time level $n$ are the same as the values at the beginning of the next time level, $n + 1$.

Energy conservation is then achieved for the discrete form by setting the test functions as the variational derivatives of the conservation equation (for periodic boundary conditions) of the form 

$$\frac{\partial H_h}{\partial u_h} \frac{(u_h^{n+1} - u_h^n)}{\Delta t} + \frac{\partial H_h}{\partial h_h} \frac{(h_h^{n+1} - h_h^n)}{\Delta t} = \frac{dH_h}{dt} = 0.$$ 

(11)

The above relation holds due to the skew-symmetry of the spatial discretisation, and the exact temporal integral of the variational derivatives, such that the temporal chain rule above is preserved discretely [12].

In addition to the energy, the spatially discrete shallow water equations may also conserve potential enstrophy,

$$Z_h = \int h_h \frac{q_h^2}{2} d\Omega.$$ 

(12)

This is achieved by recalling the compatible mappings supported by the De-Rham complex in [4] and setting $v_h = \nabla \cdot \psi_h$ in (5a) (for $\psi_h \in V_0$ and $v_h \in V_1$) [4]. Since the De-Rham complex further ensures that $\nabla \cdot \nabla = 0$ is preserved discretely, and recalling (8), (using the fact that $f_h$ does not vary with time) and (5b) this implies a potential vorticity conservation equation (for periodic boundary conditions) of the form [4]

$$\int \psi_h \frac{\partial h_h q_h}{\partial t} d\Omega + \int \psi_h \nabla \cdot (q_h F_h) d\Omega = 0 \quad \forall \psi_h \in V_0.$$ 

(13)

Since the Coriolis term is independent of time, the vorticity, $\omega_h = h_h q_h - f_h$ is conserved by the above expression for a choice of $\psi_h = 1$.

Potential enstrophy conservation may be derived by instead setting $\psi_h = q_h$ in (13), and recalling the discrete continuity equation (5b) [4, 14]. However this may be more generally derived by regarding the potential enstrophy as an additional invariant of the Hamiltonian system, or Casimir, for which conservation is ensured due to the fact that its variational derivatives are part of a null space for the skew-symmetric operator in (9). To see this we first compute the variational derivative with respect to the velocity as

$$\int \psi_h \frac{\delta Z_h}{\delta u_h} d\Omega = \left(\frac{\delta H_h}{\delta u_h}\right)^\top \frac{\delta Z_h}{\delta q_h}.$$ 

(14)

In order to describe these variational derivatives we introduce the additional linear operators $R : V_0 \to V_1'$ as $R\psi_h := \langle \nabla^+ \psi_h, \cdot \rangle$ and $H_0(\psi_h) : V_0 \otimes V_2 \to V_0'$ as $H_0(\psi_h) := \langle \phi_h \psi_h, \cdot \rangle$. Following [4], the variational derivative of the potential vorticity $q_h$ with respect to the velocity $u_h$ is given as the matrix

$$\int \psi_h h_h \frac{\delta q_h}{\delta u_h} d\Omega = -\int \nabla^+ \psi_h \cdot u_h d\Omega \Rightarrow \frac{\delta q_h}{\delta u_h} = -H_0^{-1}(h_h, R^\top u_h)$$ 

(15)

and the variational derivative of the functional $Z_h$ with respect to $q_h$ returns the vector

$$\int \psi_h \frac{\delta Z_h}{\delta q_h} d\Omega = \int \psi_h h_h q_h d\Omega \Rightarrow \frac{\delta Z_h}{\delta q_h} = M_h^{-1} H_0(h_h, q_h).$$ 

(16)

Combining (15), (16) into (14), the variational derivative of $Z_h$ with respect to $u_h$ in $V_1$ is given as

$$\frac{\delta Z_h}{\delta u_h} = -M^{-1} R H_0^{-1}(h_h, H_0(h_h, q_h)) = -M^{-1} R q_h.$$ 

(17)

Introducing the operator $Q : V_0 \times V_0 \to V_2'$ as $Q(\psi_h, \chi_h) := \langle \phi_h \chi_h, \cdot \rangle$, the variational derivative of the potential enstrophy with respect to the fluid depth in $V_2$ is similarly given as

$$\frac{\delta Z_h}{\delta h_h} = \frac{1}{2} M_z^{-1} Q(q_h, q_h).$$ 

(18)
Multiplying the skew-symmetric operator in (9) by the vector

\[ \begin{bmatrix} \frac{\delta Z_h}{\delta u_h}, & \frac{\delta Z_h}{\delta v_h} \end{bmatrix}^T = \left[ -q_h R^T M_1^{-1}, \frac{1}{2} (q_h, q_h) Q^T M_2^{-1} \right] \]

then gives

\[ -q_h R^T M_1^{-1} \left( C(\cdot, q_h) - D^T \right) + \frac{1}{2} (q_h, q_h) Q^T M_2^{-1} D \]

(20a)

\[ \begin{align*}
&= -\nabla^+ q_h C(\cdot, q_h) + \left( D M_1^{-1} R q_h \right)^T + \frac{q_h^2}{2} D \\
&= \int q_h v_h : \nabla q_h \, d\Omega + \int \phi_h \nabla \cdot \nabla^+ q_h \, d\Omega + \int \frac{q_h^2}{2} \nabla \cdot v_h \, d\Omega \\
&= \int \nabla \left( \frac{q_h^2}{2} \right) v_h \, d\Omega + \int q_h^2 \nabla \cdot v_h \, d\Omega = \int \nabla \left( \frac{q_h^2}{2} \right) \, d\Omega = 0. 
\end{align*} \]

(20b)

(20c)

(20d)

Where in the last line we have recalled the discrete property of the compatible bases that \( \nabla \cdot \nabla^+ := 0 \), as well as the assumption of periodic boundary conditions. Note that the last line above is contingent on the discrete preservation of the chain rule as

\[ \int q_h \nabla(q_h) : v_h \, d\Omega := \int \frac{1}{2} \nabla(q_h^2) : v_h \, d\Omega. \]

(21)

which only holds for exact integration [14], and so is not strictly preserved for a trigonometric Jacobian on the surface of the sphere involving transcendental functions. Now that the spatial terms have been shown to cancel for the discrete form of the potential enstrophy evolution equation, we are left with the temporal chain rule expansion in analogy to (11) as

\[ \left( \frac{\delta Z_h}{\delta u_h} \right) + \left( \frac{\delta Z_h}{\delta h_n} \right) \frac{h_n}{\Delta t} \frac{d}{dt} \frac{d Z_h}{d h_n} = \frac{d}{dt} \int \frac{h_n q_h^2}{2} \, d\Omega = 0. \]

(22)

2.2. Exact time integration of potential enstrophy

In this section new temporal formulations of the potential vorticity are introduced by which the potential enstrophy is integrated exactly across the time levels. Doing so leads to enhanced stability, such that we are able to run our simulations of two-dimensional turbulence at low Mach number without stabilisation.

Since we do not explicitly solve the advection equation for the potential vorticity [13], there is no enforcement of continuity of \( q_h \) between time levels. Rather this is diagnosed from (8). Integrating both sides of (8) with respect to \( q_h \) gives

\[ \int h_n q_h^2 \, d\Omega = -2 \int \nabla^+ q_h : u_h \, d\Omega + 2 \int q_h f_h \, d\Omega. \]

(23)

The second order integral of the above expression across the time level from \( t^r \) to \( t^{r+1} \) for piecewise linear in time \( q_h \), \( u_h \) and \( h_n \) yields a cubic temporal polynomial on the left hand side, and a quadratic on the right. Both of these may be integrated exactly using Simpson’s rule, as

\[ 2 Z_h := \int \frac{3}{2} h_n^3 (q_h^{n+1})^2 + \frac{1}{2} h_n (q_h^{n+1})^2 (h_n^2 + h_n^{n+1}) q_h^n q_h^{n+1} + \frac{1}{2} h_n^{n+1} (q_h^n)^2 + \frac{3}{2} h_n^{n+1} (q_h^{n+1})^2 \, d\Omega \]

(24a)

\[ = - \frac{1}{3} \int \nabla^+ q_h : (2u_h^n + u_h^{n+1}) + \nabla^+ q_h^{n+1} : (u_h^n + 2u_h^{n+1}) \, d\Omega + \int (q_h^n + q_h^{n+1}) f_h \, d\Omega. \]

(24b)

Differentiating with respect to \( q_h^n \) and \( q_h^{n+1} \) leads to the coupled system for the solution of the potential vorticity at both time levels

\[ \begin{bmatrix} \frac{1}{2} H_0(\cdot, 3h_n^n + h_n^{n+1}) \\
\frac{1}{2} H_0(\cdot, h_n^n + h_n^{n+1}) \\
\frac{1}{2} H_0(\cdot, h_n^n + 3h_n^{n+1}) \end{bmatrix} \begin{bmatrix} \frac{1}{2} H_0(\cdot, 3h_n^n + h_n^{n+1}) \\
\frac{1}{2} H_0(\cdot, h_n^n + h_n^{n+1}) \end{bmatrix} \begin{bmatrix} q_h^n \\
q_h^{n+1} \end{bmatrix} = \begin{bmatrix} -\frac{1}{2} R^T (2u_h^n + u_h^{n+1}) + M_0 f_h \\
-\frac{1}{2} R^T (2u_h^n + u_h^{n+1}) + M_0 f_h \end{bmatrix} \]

(25)
where as before $\mathbf{M}_0 : \mathbb{V}_0 \to \mathbb{V}_0'$ and is given as $\mathbf{M}_0\varphi_h := \langle \varphi_h, \cdot \rangle$. The above system is linear in $q_h^k$, $q_h^{k+1}$, and may be solved at each nonlinear iteration of (9). We then compute the mean potential vorticity across the time level simply as $\overline{q}_h = (q_h^k + q_h^{k+1})/2$.

Alternatively, we may represent $\overline{q}_h$ as being piecewise constant in time, for which the potential enstrophy is exactly integrated over the time level as

$$2\mathcal{Z}_h := \frac{1}{2} \int (h_h^k + h_h^{k+1})\overline{q}_h^2 d\Omega = -\int \nabla \overline{q}_h \cdot (u_h^k + u_h^{k+1}) d\Omega + 2 \int \overline{q}_h f_h d\Omega. \tag{26}$$

In this case the potential vorticity is more simply diagnosed from the piecewise linear in time $u_h, h_h$ by differentiating with respect to $\overline{q}_h$ as

$$H_h(\overline{q}_h, h_h^k + h_h^{k+1}) = -R^T(u_h^k + u_h^{k+1}) + 2\mathbf{M}_0 f_h. \tag{27}$$

We stress that while the above formulations yield exact temporal integration of potential enstrophy across the time level, they do not ensure exact conservation between time levels, such that unlike the energy, potential enstrophy will still not be exactly conserved in time.

2.3. Time integration

The resulting nonlinear problem (9), (7) and (25) or (27) is then solved using a Newton method with a constant in time approximate Jacobian [7, 19], which at each nonlinear iteration $k$ is solved for the updates $\delta u_h^k = u_h^{k+1} - u_h^k$, $\delta h_h^k = h_h^{k+1} - h_h^k$ as

$$\begin{bmatrix} \mathbf{M}_1 + 0.5\Delta t \mathbf{C}(\cdot, f) & -0.5\Delta t \mathbf{g}^T \\ 0.5\Delta t H \mathbf{D} & \mathbf{M}_2 \end{bmatrix} \begin{bmatrix} \delta u_h^k \\ \delta h_h^k \end{bmatrix} = - \begin{bmatrix} \mathbf{R}_u^k \\ \mathbf{R}_h^k \end{bmatrix} \tag{28}$$

where $H$ is the mean fluid depth and $k$ is the estimate of the solution at time level $n+1$ at the current Newton iteration.

Note that this constant Jacobian omits nonlinear terms due to variations in the potential vorticity, mass flux and Bernoulli potential. Since the vorticity field varies only slowly with time compared to the gravity waves, and we consider only weakly hyperbolic flow regimes for which variations in $h_h$ are small with respect to $H$, this is sufficient to achieve numerical convergence. The residuals at iteration $k$ are given via (9) as:

$$\begin{align*}
\mathbf{R}_u^k &= \mathbf{M}_1(u_h^k - u_h^k) + \Delta t \mathbf{C} \overline{F}_h, \overline{q}_h - \Delta t \mathbf{g}^T \overline{P}_h, \tag{29a} \\
\mathbf{R}_h^k &= \mathbf{M}_2(h_h^k - h_h^k) + \Delta t \mathbf{D} \overline{F}_h. \tag{29b}
\end{align*}$$

Note that at each Newton iteration $k$, prior to the evaluation of the solution increments $\delta u_h^k, \delta h_h^k$, we must first evaluate the variational derivatives, $\overline{F}_h, \overline{P}_h$, as well as the potential vorticity $\overline{q}_h$ (setting $k = n + 1$ as a proxy at each iteration). The full solution procedure at each nonlinear iteration $k$ therefore follows as:

1. Compute the exact integral of the variational derivatives $\overline{F}_h, \overline{P}_h$ across the time level $n + 1$ and the approximation of time level $n + 1$ at iteration $k$ via (10).

2. Compute the second order integral of the potential vorticity $q_h$ as either:
   (a) A time centered average $q_h^{n+1/2} = (q_h^n + q_h^{n+1})/2$, where $q_h^n$ and $q_h^{n+1}$ are evaluated instantaneously via (8).
   (b) Exact piecewise constant integration of $\overline{q}_h$ over the time level via (27).
   (c) Exact piecewise linear integration of $\overline{q}_h$ over the time level via (25).

3. Evaluate the residuals $\mathbf{R}_u^k, \mathbf{R}_h^k$ via (29).

4. Solve for the solution increments $\delta u_h^k, \delta h_h^k$ via (28).

5. Update the solutions as $u_h^{k+1} = u_h^k + \delta u_h^k, h_h^{k+1} = h_h^k + \delta h_h^k$, and increment $k \to k + 1$.

6. Terminate the Newton iteration if $k > k_{max}$, for maximum iteration number $k_{max}$, or if $|\delta u_h^k|/|u_h^k| < \epsilon_{sol}$ and $|\delta h_h^k|/|h_h^k| < \epsilon_{sol}$, where $\epsilon_{sol}$ is some specified solver tolerance.
3. Potential vorticity upwinding

3.1. The anticipated potential vorticity method (APVM)

Energy conservation is preserved for any choice of \( q_h \) in (5a), since the term \( \int \nu_h q_h \Omega_h \, d\Omega = 0 \) for \( \nu_h = F_h \) is in any case skew-symmetric, as shown in (9). Consequently \( q_h \) may be upwinded as a means of damping small scale oscillations without breaking energy conservation. Perhaps the most straight-forward form of upwinding is the anticipated potential vorticity method [1, 4], for which the potential vorticity is replaced in (5a) by its upstream value

\[
q_h = \tau u_h \cdot \nabla q_h, \tag{30}
\]

where \( \tau \) is an upwinding timescale parameter. In the simplest case, \( \tau \) is typically a constant of the same order as the time step, \( O(\Delta t) \), however it may also include additional terms that scale with the advective term or other physics [20]. Substitution of (30) into (5a), and then following the same procedure used to derive the flux form advection equation for \( q_h \) in (13) [3], results in a modified form of the potential vorticity advection equation (13) as

\[
\int \psi_h \frac{\partial q_h}{\partial t} + \psi_h \nabla \cdot \left( F_h \left( q_h - \tau u_h \cdot \nabla q_h \right) \right) \, d\Omega = 0 \quad \forall \psi_h \in \mathcal{V}_0. \tag{31}
\]

Note that this expression is not consistent with respect to (13), such that it will converge to a different solution for \( q_h \) with increased resolution. Again setting \( \psi_h = q_h \), the analogous form of (22) is given as

\[
\int \frac{\partial}{\partial t} \left( \frac{h_q q_h^2}{2} \right) d\Omega + \int \tau h_q (u_h \cdot \nabla q_h)^2 d\Omega = 0. \tag{32}
\]

From this we see that the APVM upwinding results in the addition of a symmetric positive definite dissipation term to the potential enstrophy evolution that acts to always remove potential enstrophy from the system for \( \tau > 0 \).

3.2. The streamwise upwind Petrov-Galerkin method (SUPG)

As a consistent alternative to the APVM [30], we may instead replace the potential vorticity by a corrected upwinded formulation as [6, 7]

\[
q_h = \tau u_h \cdot \nabla q_h \tag{33}
\]

for which

\[
\int \psi_h \frac{\partial h_q q_h}{\partial t} + \psi_h \nabla \cdot \left( F_h \left( q_h - \tau u_h \cdot \nabla q_h \right) \right) \, d\Omega = 0 \quad \forall \psi_h \in \mathcal{V}_0. \tag{34}
\]

Rearranging this expression, and again recalling the continuity equation (5b) gives

\[
\int h_q \left( \psi_h + \tau u_h \cdot \nabla \psi_h \right) \left( \frac{\partial q_h}{\partial t} + u_h \cdot \nabla q_h \right) \, d\Omega = 0 \quad \forall \psi_h \in \mathcal{V}_0. \tag{35}
\]

This consistent modification of the trial function constitutes the SUPG formulation [2, 5]. The corresponding potential enstrophy evolution equation is given for \( \psi_h = q_h \) as

\[
\int \frac{\partial}{\partial t} \left( \frac{h_q q_h^2}{2} \right) d\Omega + \int \tau h_q (u_h \cdot \nabla q_h)^2 d\Omega + \int \tau h_q \left( \frac{\partial q_h}{\partial t} \right) (u_h \cdot \nabla q_h) d\Omega = 0. \tag{36}
\]

The second term in (36) is identical to that in (32), ensuring that potential enstrophy is dissipated via the same mechanism as for APVM. Since \( q_h \) is materially advected, we have that \( \frac{\partial q_h}{\partial t} \approx -u_h \cdot \nabla q_h \), such that the third term acts as a backscatter term to inject potential enstrophy back into the system, ensuring a richer representation of grid scale turbulence than for the APVM. However since this term is not sign definite it will not fully counter balance the potential enstrophy dissipation of the second term, ensuring the net dissipation of the overall scheme.

Note that we have made no assumption as to the form of \( \tau \), other than that it is \( > 0 \). This may be set as a constant value, or as a spatially and temporally varying field which scales with both the time derivative and the advection term.
3.3. Downwinded trial functions

As an alternative to these traditional approaches, one may effectively upwind the potential vorticity by downwinding the reference element trial functions in the case of weak form differential operators \([9]\), or upwinding the test functions in the case of strong form differential operators \([11, 12]\). In either case, this may be achieved by moving the location of the quadrature point, \(\xi\) at which the reference element basis function, \(\hat{l}_i(\xi)\) is evaluated, provided that \(\hat{l}_i(\xi); i = 1, \ldots, p\) span a finite element space of polynomial degree \(p\) that is \(C^0\) continuous in the direction of the flow (which is the case in both dimensions for the space \(\mathbb{V}_0 \subset H^1(\Omega)\)).

For the downwinded reference element trial functions, these are evaluated as \(\hat{l}_i^d(\xi; \hat{u}(\xi)) = \hat{l}_i(\xi - \tau \hat{u}(\xi))/|J|\), where \(\tau\) is again some time scale parameter, \(\hat{u}\) is the velocity in reference element coordinates, and \(|J|\) is the Jacobian determinant of the geometrical map, \(\Phi\) \([21]\), evaluated at \(\xi\). Conversely, the upwinded test functions may be evaluated as \(\hat{l}_i^u(\xi; \check{u}(\xi)) = \hat{l}_i(\xi + \tau \hat{u}(\xi))/|J|\). For a trial (resp. test) function of degree \(p\) may be expanded as

\[
\begin{align*}
\hat{l}_i^d(\xi; \hat{u}(\xi)) &= \hat{l}_i(\xi - \tau \hat{u}(\xi))/|J| - \hat{l}_i(\xi) + \frac{(\tau \hat{u}(\xi))^2}{2|J|^2} d\hat{l}_i(\xi) + \frac{(\tau \hat{u}(\xi))^3}{6|J|^3} d^2\hat{l}_i(\xi) + \cdots + \frac{(-\tau \hat{u}(\xi))^p}{p!|J|^p} d^p\hat{l}_i(\xi), \\
\hat{l}_i^u(\xi; \check{u}(\xi)) &= \hat{l}_i(\xi + \tau \hat{u}(\xi))/|J| - \hat{l}_i(\xi) + \frac{(\tau \hat{u}(\xi))^2}{2|J|^2} d\hat{l}_i(\xi) + \frac{(\tau \hat{u}(\xi))^3}{6|J|^3} d^2\hat{l}_i(\xi) + \cdots + \frac{(+\tau \hat{u}(\xi))^p}{p!|J|^p} d^p\hat{l}_i(\xi).
\end{align*}
\]

In two dimensions the downwinded trial/upwinded test functions may be expressed in reference space as

\[
\begin{align*}
\hat{\psi}^d_i(\xi; \hat{u}) &= \hat{\psi}^d_i(\xi; \hat{u}(\xi)) \otimes \hat{F}_{\hat{u}}(\hat{\xi}^d; \hat{\eta}^d), \\
\hat{\psi}^u_i(\xi; \check{u}) &= \hat{\psi}^u_i(\xi; \check{u}(\xi)) \otimes \hat{F}_{\check{u}}(\hat{\xi}^u; \hat{\eta}^u),
\end{align*}
\]

where \(\hat{\xi} = (\hat{\xi}, \hat{\eta})\) are the two dimensional local element coordinates, \(\hat{u} = (\hat{u}, \hat{v})\) are the two dimensional velocity components in the reference element and \(h = j(p + 1) + i\) is the index of the two dimensional tensor product basis function. These downwinded (resp. upwinded) trial (resp. test) functions may then be pushed forward into physical space as

\[
\begin{align*}
\psi_i^d(x; \hat{u}(\xi)) &= \left[ \hat{\psi}_h\left(\xi - \tau \hat{u}(\xi)/|J|\right) \right] \circ \Phi^{-1}(x), \\
\psi_i^u(x; \check{u}(\xi)) &= \left[ \hat{\psi}_h\left(\xi + \tau \hat{u}(\xi)/|J|\right) \right] \circ \Phi^{-1}(x),
\end{align*}
\]

where \(x\) are the global coordinates. The downwinded form of the potential enstrophy is then given in physical coordinates by \(q^d_i(x)\).

Since it is the trial functions that are downwinded, the above expansion enters both the flux term and the temporal derivative, giving the analogue of \([13]\) as

\[
\int \psi_i \frac{\partial h q^d_i}{\partial t} + \psi_k \nabla \cdot (F d q^d_k) \, d\Omega = 0 \quad \forall \psi_b \in \mathbb{V}_0.
\]

Since the downwinded correction to the potential vorticity in \([38a]\) can be expressed as a Taylor series correction to the static trial functions, we label this as \(a' = q^d_h - q_h\). Rearranging and recalling the continuity equation then gives

\[
\int \psi_i h_b \left( \frac{\partial h}{\partial t} + u_b \cdot \nabla q_h \right) \, d\Omega + \int \psi_i h_b \left( \frac{\partial}{\partial t} + u_b \cdot \nabla \right) q^d_i \, d\Omega = 0 \quad \forall \psi_b \in \mathbb{V}_0.
\]

While the additional trial function corrections presented above are not consistent, if instead the test functions are upwinded using the same approach, as has been done previously for the stabilisation of potential temperature in the 3D compressible Euler equations \([12]\), then the resulting stabilisation is indeed consistent. The resulting potential enstrophy evolution equation for the downwinded trial functions is given as

\[
\int \frac{\partial}{\partial t} \left( \frac{h q^d_i}{2} \right) \, d\Omega + \int h_i q^d_i \left( \frac{\partial h}{\partial t} + u_b \cdot \nabla q^d_i \right) \, d\Omega = 0.
\]
From \( (37a) \) we have to a first approximation that
\[
q_h' \approx -\tau u_h \cdot \nabla q_h.
\]
If we further assume periodic boundary conditions in time as well as space for the grid scale dynamics driven by the potential enstrophy cascade, then we may apply integration by parts to the material transport operator
\[
L = \frac{\partial}{\partial t} + u_h \cdot \nabla
\]
in the second term of \( (42) \), resulting in an expression equivalent to \( (36) \). We therefore anticipate that for the small scales on which the damping term operates that the downwindind trial function formulation should yield similar results as for the SUPG scheme, and any consistency errors will be small.

As stated above, the downwinded trial functions are applied both when the potential vorticity is diagnosed, resulting in a downwind correction to the time derivative in the advection equation, and to the rotational term in the momentum equation, resulting in a downwinded correction to the flux term in the advection equation. The fully discrete diagnostic \( (8) \) and residual \( (29a) \) expressions are therefore expressed for the downwinded trial functions as
\[
H_0(q_h^d, h_h) = -R^\top u_h + M_0 f_h, \tag{43}
\]
\[
M_1 R^k u = M_1 (u_h^k - u_h^n) + \Delta t C(F_{\bar{h}, q_{\bar{h}}}) - \Delta t D^\top \bar{P}_h. \tag{44}
\]

4. Results

4.1. Nonlinearly converged solutions

In order to quantify the differences between the APVM, SUPG and downwinded trial function formulations, these are compared in the context of a shear flow instability of a barotropic jet, as triggered by a small initial perturbation in the otherwise geostrophically balanced depth field \( [13] \), on a cubed sphere using polynomials of degree \( p = 3 \) for the representation of the potential vorticity \( [22] \). The test case was run for 20 days using \( 6 \times 32 \times 32 \) elements and 8 point Gauss-Lobatto-Legendre quadrature and a time step of 360.0s. In the first set of tests the implicit nonlinear solver was converged to a tolerance of \( 10^{-14} \), using exact temporal integration of the variational derivatives \( [7, 12, 15] \), allowing for a machine precision error in energy conservation. In each case the upwinding parameter was set to a value of \( \tau = \Delta t/2 = 180.0s \). For the results presented in this section and the next we compute the potential vorticity not through the exact time integration of potential enstrophy across the time level as in \( (25) \) or \( (27) \) but rather with a simple second order in time averaging of the potential vorticity as \( q_h^{n+1/2} = (q_h^n + q_h^k)/2 \) at each Newton iteration \( k \), where \( q_h^n \) and \( q_h^k \) are computed instantaneously from \( (8) \) using \( (u_h^n, h_h^n) \) and \( (u_h^k, h_h^k) \) respectively, and without the temporal cross terms that would arise from the evaluation of \( q_h \) via \( (25) \) or \( (27) \).

![Figure 1: Vorticity field (northern hemisphere) for the Galewsky test case at day 7 using APVM (left), SUPG (center) and downwinded trial functions (right) for the converged solutions.](image-url)
Figures 1 and 2 show the vorticity field in the northern hemisphere for the three upwinding formulations at days 6 and 20 respectively. In both cases the SUPG and downwinded trial function schemes look very similar, as suggested by our analysis in the previous section. However the APVM results exhibit excessive dissipation of the potential enstrophy at day 20, due to the symmetric definite correction to the potential enstrophy evolution that this implies (32). The difference between APVM and the other schemes is also evident at day 7. This is due to the fact that the excessive damping of the potential enstrophy means the nonlinear shear flow instability is triggered slightly later.

The conservation properties (energy and potential enstrophy) are given in Fig. 3. In all cases the energy conservation error is machine precision. The potential enstrophy conservation error is comparable for the SUPG and downwinded trial function formulations, reflecting a similar amount of variation in the vorticity fields, as shown in Fig. 2. However the APVM exhibits a significantly greater amount of potential enstrophy dissipation, owing to the symmetric definite nature of the correction to the potential enstrophy equation.

The mass and vorticity conservation errors are given in Fig. 4. In each case the mass conservation is exact (machine precision), while the global vorticity integral (over a sphere of radius 6371220.0m) is un-normalised and of \( O(10^{-5}) \), showing that in each case the potential vorticity stabilisation has no bearing on its conservation.
While the energy and potential enstrophy conservation errors are remarkably similar for the SUPG and downwinded trial functions, the number of iterations required to achieve convergence of the nonlinear solver differs greatly, as shown in Fig. 5. The downwinded trial function solution requires fewer iterations on average to achieve convergence than either the APVM or SUPG formulations. This is perhaps due to the additional higher order corrections in the Taylor series expansion of the downwinded trial functions \(^{37a}\). This improved solver convergence is despite the fact that the turbulent profile is almost identical to that for the SUPG formulation, as reflected in the kinetic energy spectra at day 20, as also shown in Fig. 5 and the potential vorticity field, as observed in Fig. 2. Both the SUPG and downwinded trial function kinetic energy spectra are closer to the theoretical profile for two dimensional turbulence of \(k^{-3}\) (for spherical harmonic wavenumber \(k\)).

SUPG schemes are typically run with a more sophisticated representation of \(\tau\) so that this may scale with both the time derivative and the advective term (and any other additional terms in the underlying equation \(^{20}\)). To this end the experiments were re-run with a value of \(\tau = (2/\Delta t + |u_h|/(2 \sqrt{|J|}))^{-1}\). Once more, the potential enstrophy results were remarkably similar between the SUPG and downwinded trial function schemes. However the number of iterations required to achieve convergence was reduced for both schemes, with the SUPG scheme showing the greatest improvement, such that the average number of iterations between the two schemes was almost the same over the course of the simulations, as show in Fig. 6.
Figure 6: Potential enstrophy conservation (left) and number of iterations to achieve convergence (right) using $\tau = (2/\Delta t + |u_0|/(2 \sqrt{|J|}))^{-1}$.

4.2. Finite number of nonlinear iterations

The results of the SUPG and downwinded trial function solutions are remarkably similar for the case where the nonlinear residual is converged to machine precision (at the expense of a larger number of iterations for the SUPG scheme). However, the faster convergence of the downwinded trial function formulation means that the results differ more sharply for the case where only a finite number of nonlinear iterations (two) are employed, as is customary in atmospheric models [23] for which performance is a premium concern. As for the previous section, here the potential vorticity is computed as a second order averaging of the instantaneous values at the previous time level $n$ and the new time level at Newton iteration $k$, $q_{y_{n+1/2}} = (q_{y_{n}} + q_{y_{k}})/2$, and not using the exact temporal integration of the potential enstrophy across the time level, as in (25) or (27).

Figure 7: Vorticity field (northern hemisphere) for the Galewsky test case at day 7 using APVM (left), SUPG (center) and downwinded trial functions (right) using two nonlinear iterations per time step.

As shown in Figs. 7 and 8, the results of the SUPG and downwinded trial function formulations are still remarkably similar to visual inspection at both days 6 and 20 for the case where only two nonlinear iterations are employed per time step. While the potential enstrophy errors are also very similar, as observed in Fig. 9, the energy conservation errors differ markedly, with the downwinded trial function energy conservation error being significantly smaller over
the course of the simulation. The mass and vorticity conservation errors are essentially the same as for the converged solution, as shown in Fig. [10]

This difference in the energy conservation error is also reflected in the nonlinear residual at the second iteration, as shown in Fig. [11]. This error is significantly smaller for the downwinded trial functions than the SUPG formulation, particularly at the maximum growth of the shear instability (around days 8-9). Curiously, the residual error is remarkably similar for the APVM and downwinded trial functions, despite the fact that the turbulence profile is much richer for the downwinded trial functions, as also shown for day 20 in Fig. [11]

The energy conservation and residual errors between the SUPG and downwinded trial function formulations are also compared using a spatially and temporally varying value of $\tau = (2/\Delta t + |u_h|/(2 \sqrt{|J|}))^{-1}$ in Fig. [12]. While the residual errors for the SUPG formulation are somewhat improved with respect to the constant value results given in Fig. [11], the energy conservation errors are significantly poorer than those shown for the SUPG scheme in Fig. [9]. The downwinded trial function results are similar in both cases.
Figure 10: Mass (left) and un-normalised vorticity (right) conservation using two nonlinear iterations per time step.

Figure 11: Kinetic energy spectra at day 20 (left), and residual error at the second iteration using two nonlinear iterations per time step (left).

Figure 12: Energy conservation (left) and residual errors at the second iteration (right), using two nonlinear iterations and \( \tau = (2/\Delta t + |u_h|/(2 \sqrt{\gamma}))^{-1} \).
4.3. Exact temporal integration of potential enstrophy

We also compare the energy conserving results presented in Section 4.1 with results for which potential enstrophy is exactly integrated across each time level, via the diagnosis of $\mathcal{Q}_h$ as either piecewise linear (25) or piecewise constant (27) in time. Since there is no internal dissipation of energy in space or time, and only minimal change in potential enstrophy for these configurations, any injection of potential enstrophy, such as that provided by the SUPG or downwinned trial function stabilisation schemes, will lead to instability. Consequently these formulation can only be run in either a neutral state, with no damping, or in conjunction with a symmetric positive definite damping term, such as that for the APVM. Results showing the potential enstrophy evolution for the exact potential enstrophy integration formulations are presented in Fig. 13, with these contrasted against those for the standard second order representation as shown in Fig. 3. As observed, the second order in time representation of potential vorticity lead to a potential enstrophy conservation error approximate one quarter that of the piecewise constant representation for the completely undamped case ($\tau = 0$). As previously noted, since these schemes ensure the exact temporal integration of $\mathcal{Z}_h$ across the time level, but not between time levels, while they yield greatly improved results in terms of stability and conservation, unlike energy $\mathcal{Z}_h$ is still not conserved exactly.

Figure 13: Potential enstrophy (left) and kinetic energy spectra at day 20 (right) using both inexact and exact potential enstrophy conserving time stepping. Note the different scales of the vertical axes for the stabilised configuration absolute values vs. unstabilised configuration normalised errors in the left hand plot.

As observed in Fig. 13 using the exact temporal integration of the potential enstrophy the APVM may be run stably with any choice of $\tau \geq 0$, including smaller values than those required to stabilise simulations with an inexact time integration of potential enstrophy. Using such small values of $\tau$, the APVM may yield superior results to either the SUPG or downwinned trial function formulations in terms of both conservation error and turbulent spectra.

4.4. Comparisons in a gravity wave dominated regime

While the previous test provides useful insights into the performance of the different potential vorticity upwinding schemes for flows dominated by vorticity dynamics and turbulence, it is less useful for investigating the different schemes in the context of gravity wave dominated flows. In order to compare the different schemes in this regime we apply them to a standard test case for orographically generated gravity waves [24]. The test involves a geostrophically balanced flow for a fluid of mean depth $H = 5960\text{m}$ over an isolated mountain with a profile of $b(r) = 2000 \times (1 - r/R)$, where $R = \pi/9$ and $r^2 = (\theta - \pi/6)^2 + (\lambda + \pi/2)^2$, and $\theta$ and $\lambda$ are the latitude and longitude respectively. The bottom topography is applied to the solver as an addition to the Bernoulli potential, $\mathcal{P}_h$ [40], of the form $\int g b h_d \Omega$, where $b_h$ is the discrete projection of $b$ onto $V_2$. The topography is correspondingly incorporated into the energy as $\mathcal{H}_t = \int \frac{1}{2} h \mathbf{u} \cdot \mathbf{u} + \frac{1}{2} g (h + b_h)^2 \Omega$ [19].

The different schemes were all run using $6 \times 16 \times 16$ elements using polynomials of degree $p = 3$ and 8 point quadrature with a time step of $\Delta t = 600\text{s}$ for a total of 20 days. As for the barotropic jet test configuration above, these were compared for simulations that were run to nonlinear convergence at each time step, and also for simulations using just two Newton iterations per time step. Visual inspection of the total depth $(h_b + b_h)$ and vorticity fields at day
15 showed little variation between the result for the different formulations, with the nonlinearly converged solutions being in all cases slightly sharper than the results using just two nonlinear iterations. The total depth field at day 15 using the downwinded trial function stabilisation for the nonlinearly converged solution is presented in Fig. 14.

![Figure 14: Left: total depth at day 15 for the nonlinearly converged solution of the flow over an isolated mountain test case at each time step using the downwinded trial function stabilisation. Solid contours are given from 5100m to 5900m in increments of 100m. Right: normalised total energy conservation errors using two Newton iterations and nonlinear converged solutions for the different potential vorticity upwinding schemes. Note the different vertical axes for the energy conservation error using two iterations and nonlinearly converged solutions.](image)

While the results appear visually similar, differences in the energy conservation errors can be easily discerned in Fig. 14. As expected, in all cases energy is conserved to machine precision when the Newton solver is run to convergence. When using only two Newton iterations per time step the SUPG method leads to the largest energy loss, while the exact computation of the potential enstrophy across the time level, via (27), leads to long term energy growth. As for the previous test case all formulations other than the exact integral of potential enstrophy across the time level use a simple time centered formulation of $q_n^{n+1} = (q_n^n + q_k^n)/2$, with $q_n^n$ and $q_k^n$ computed instantaneously via (8). Long time energy growth is also slightly perceptible for the APVM and downwinded trial function solutions, suggesting that these methods are perhaps slightly under-damped.

The potential enstrophy conservation errors are presented in Fig. 15, in normalised absolute value form on a logarithmic plot. All solutions exhibit a decay of potential enstrophy with time, with the exception of the two iteration solution using exact integration of potential enstrophy across the time level, for which this grows with time, suggesting that for two iterations the solution will ultimately go unstable. Once more the APVM method is most dissipative, using both two Newton iterations or a nonlinearly converged solution. Results are nearly identical for the SUPG and downwinded trial function solutions for nonlinearly converged solutions, while for two iterations the SUPG method is slightly more dissipative. As for the previous test case, exactly integrating the potential enstrophy across the time level with a converged Newton iteration at each time step leads to greatly improved potential enstrophy conservation errors, which are steady throughout the simulation at $O(10^{-10})$.

Since the potential enstrophy shows no discernible decrease with time when this is exactly integrated across the time level, its turbulent cascade to grid scales will introduce some amount of noise into the solution. In Fig. 15 we give the normalised potential enstrophy conservation errors as a function of time with increased spatial and temporal resolution. These errors decrease quadratically (the order of the time stepping scheme), suggesting that while there will be some degree of noise for these solutions due to the turbulent cascade of potential enstrophy in the absence of dissipation, this noise nevertheless decreases with resolution. This result is visually confirmed in Fig. 16 which gives the vorticity field at day 15 for the flow over the isolated mountain test case using resolutions of $6 \times 8^2$ elements with $\Delta t = 1200s$ and $6 \times 32^2$ elements with $\Delta t = 300s$, where it is clearly observed that the higher resolution result is also smoother at the grid scale. As an aside, we also note that if the potential enstrophy does not decrease with time for two dimensional flows where this cascades to the grid scale, this is most likely indicative of grid scale noise, which may be deemed unacceptable for practical applications.

As for the previous test case, mass and vorticity are exactly conserved in all cases. These results are not presented.
here. In terms of the total number of Newton iterations for the case where the different configurations were run to convergence at each time step, these were remarkably similar, averaging 23.27 iterations for the APVM scheme, and 23.26 iterations for the other formulations. The results were also very similar between the different formulations for the residual error at the second iteration when run with just two Newton iterations. The close similarity of these results is perhaps unsurprising, since the upwind stabilisation applied here is specifically targeting the potential vorticity transport, and this has less overall effect on the dynamics for the gravity wave dominated test case than it does for the previous shear instability test case.

Figure 15: Left: normalised absolute values of the potential enstrophy conservation errors using two Newton iterations and nonlinear converged solutions for the different potential vorticity upwinding schemes for the flow over an isolated mountain test case. Note that these are decaying for all schemes, with the exception of the two iteration $Z$ exact solution. Right: normalised absolute value of the potential enstrophy conservation error for the nonlinear converged solution as a function of resolution for the piecewise constant in time exact integration of $Z$ across the time level via (27).

Figure 16: Vorticity field at day 15 using $6 \times 8^2$ elements and $\Delta t = 1200s$ (left) and $6 \times 32^2$ elements and $\Delta t = 300s$ (right) for the flow over an isolated mountain test case using piecewise constant in time exact integration of $Z$ across the time level.

5. Conclusions

Different forms of potential vorticity upwinding are analysed and compared for a high order mixed finite element discretisation of the rotating shallow water equations on the sphere. These include the well known APVM and SUPG methods, as well as a more recently proposed method by which the basis functions are evaluated at downstream locations in reference element coordinates. Both analysis and numerical experiments show that the reference element
downwinding and SUPG methods are clearly superior to the APVM method in terms of their turbulent profiles and potential enstrophy conservation. While the SUPG and downwinded trial function formulations are very similar in terms of both their potential enstrophy conservation and turbulent spectra, the downwinded trial functions exhibit better energy conservation and smaller residual errors for a finite number of nonlinear iterations for both constant and non-constant values of the upwinding parameter. For a fully converged solution the downwinded trial functions exhibit faster convergence if a constant upwinding parameter is used, however the convergence rates are more comparable for a non-constant upwinding parameter.

One possible explanation for the improved results of the downwinded trial functions is that while the potential vorticity is diagnosed from the prognostic variables \(\mathbf{u}, h\) in the formulation presented here, it may alternatively be represented via a material advection equation [13]. By applying a higher order representation of the upwinding, we are effectively providing a more accurate approximation of where the potential vorticity departure point would be located at some previous time, were this to be represented as a Lagrangian (or semi-Lagrangian) variable. The downwinded trial functions therefore take more account of the material nature of the potential vorticity.

In addition to the comparison of upwind stabilisation schemes, we also present new temporal formulations of the potential vorticity diagnostic equation that imply the exact integration of potential enstrophy across the time level (but not between time levels) for both piecewise linear and piecewise constant (in time) potential vorticity. These temporal discretisations are observed to be almost neutrally stable, and so allow for the stable simulation of a mature turbulent state without any form of dissipation. When run in conjunction with the APVM using values of \(\tau\) \(\mathcal{O}(100)\) times smaller than those typically required, these formulations exhibit superior conservation properties and turbulence profiles than those observed for either the SUPG or downwinded trial function formulations when run using a simple time centered (inexact) formulation for the potential vorticity and a more moderate value of the upwinding parameter.

Results for a standard test case for flow over an isolated mountain (for which the solution is well resolved at lower resolution than for the geostrophic turbulence test case) using exact integration of potential enstrophy across the time level show that potential enstrophy conservation errors decrease with the second order accuracy of the time stepping scheme. As such the grid scale noise due to the lack of potential enstrophy damping in this formulation reduces with increased resolution, which is also confirmed by visual inspection of the vorticity field at different resolutions.

We end by noting that while the upwind stabilisation of the potential vorticity has been the main subject of this article, these approaches are equally applicable to other material variables that appear in the skew-symmetric operators of Hamiltonian systems, as has been previously demonstrated for the potential temperature in the case of the 3D compressible Euler equations [8][12].

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**References**

[1] R. Sadourny, C. Basdevant, Parameterization of Subgrid Scale Barotropic and Baroclinic Eddies in Quasi-geostrophic Models: Anticipated Potential Vorticity Method, J. Atmos. Sci. 42 (1985) 1353–1363
[2] A. N. Brooks, T. J. R. Hughes, Streamline upwind/Petrov-Galerkin formulations for convection dominated flows with particular emphasis on the incompressible Navier-Stokes equations, Comput. Meth. Appl. Mech. Engrg. 32 (1982) 199–259
[3] T. J. R. Hughes, G. R. Feijoo, L. Mazzei, J.-B. Quincy, The variational multiscale method—a paradigm for computational mechanics, Comput. Methods Appl. Mech. Engrg. 166 (1998) 3–24
[4] A. T. T. McRae, C. J. Cotter, Energy- and enstrophy conserving schemes for the shallow water equations, based on mimetic finite elements, Q. J. R. Meteorol. Soc. 140 (2014) 2223–2234.
[5] A. Natale, C. J. Cotter, Scale-selective dissipation in energy-conserving finite-element schemes for two-dimensional turbulence, Q. J. R. Meteorol. Soc. 143 (2017) 1734–1745.
[6] A. Natale, J. Shipton, C. J. Cotter, Compatible finite element spaces for geophysical fluid dynamics, Dyn. Stat. Climate Sys. 1 (2016) 1–31.
[7] W. Bauer, C. J. Cotter, Energy-enstrophy conserving compatible finite element schemes for the rotating shallow water equations with slip boundary conditions, J. Comp. Phys. 373 (2018) 171–187.
[8] G. A. Wimmer, C.J. Cotter, W. Bauer, Energy conserving SUPG methods for compatible finite element schemes in numerical weather prediction, SMAI journal of computational mathematics, 7 (2021), 267–300
[9] R. Brecht, W. Bauer, A. Biblo, F. Gay-Balmaz, S. MacLachlan, Selective decay for the rotating shallow-water equations with a structure-preserving discretization, Physics of Fluids 33 (2021) 116604.
[10] S. Marras, F. X. Giraldo, A parameter-free dynamic alternative to hyper-viscosity for coupled transport equations: Application to the simulation of 3D squall lines using spectral elements, J. Comp. Phys. 283 (2015) 360–373.
[11] D. Lee, Petrov-Galerkin flux upwinding for mixed mimetic spectral elements, and its application to geophysical flow problems, Comput. Math. Appl. 89 (2021) 68–77
[12] D. Lee, A. Palha, Exact spatial and temporal balance of energy exchanges within a horizontally explicit/vertically implicit non-hydrostatic atmosphere, J. Comp. Phys. 440 (2021) 110432
[13] J. Galewsky, R. K. Scott, L. M. Polvani, An initial-value problem for testing numerical models of the global shallow water equations, Tellus 56A (2004) 429–440
[14] D. Lee, A. Palha, M. Gerritsma, Discrete conservation properties for shallow water flows using mixed mimetic spectral elements, J. Comp. Phys. 357 (2018) 282–304
[15] C. Eldred, T. Dubos, E. Kritsikis, A quasi-Hamiltonian discretization of the thermal shallow water equations, J. Comp. Phys. 379 (2019) 1–31
[16] E. Celledoni, V. Grimm, R. I. McLachlan, D. I. McLaren, D. I. O’Neale, B. Owren, G. R. W. Quispel, Preserving energy resp. dissipation in numerical PDEs using the “average vector field” method, J. Comput. Phys. 231 (2012) 6770–6789.
[17] D. Cohen, E. Hairer, Linear energy-preserving integrators for Poisson systems, BIT Numer. Math. 51 (1) (2011) 91–101.
[18] D. Lee, An energetically balanced, quasi-Newton integrator for non-hydrostatic vertical atmospheric dynamics, J. Comp. Phys. (2021) 109988.
[19] G. A. Wimmer, C.J. Cotter, W. Bauer, Energy conserving upwinded compatible finite element schemes for the rotating shallow water equations, J. Comp. Phys. 401 (2020) 109016
[20] J. Ed Akin, T. E. Tezduyar, Calculation of the advective limit of the SUPG stabilization parameter for linear and higher-order elements, Comput. Methods Appl. Mech. Engrg. 193 (2004) 1909–1922
[21] M. E. Rognes, D. A. Ham, C. J. Cotter, A. T. T. McRae, Automating the solution of PDEs on the sphere and other manifolds in FEniCS 1.2, Geosci. Model. Dev. 6 (2013) 2099–2119
[22] D. Lee, A. Palha, A mixed mimetic spectral element model of the rotating shallow water equations on the cubed sphere, J. Comp. Phys. 375 (2019) 240–262
[23] T. Melvin, T. Benacchio, B. Shipway, N. Wood, J. Thuburn, C. Cotter, A mixed finite-element, finite-volume, semi-implicit discretisation for atmospheric dynamics: Cartesian geometry, Q. J R. Meteorol. Soc. (2019) 1–19.
[24] D. L. Williamson, J. B. Drake, J. J. Hack, R. Jakob, P. N. Swarztrauber, A standard test set for numerical approximations to the shallow water equations in spherical geometry, J. Comp. Phys. 102, (1992) 211–224.