Conservative Numerical Schemes with Optimal Dispersive Wave Relations: Part II. Numerical Evaluations

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Received: 25 June 2021 / Revised: 4 March 2022 / Accepted: 17 April 2022 / Published online: 12 July 2022
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Abstract
A new energy and enstrophy conserving scheme (EEC) for the shallow water equations is proposed and evaluated using a suite of test cases over the global spherical or bounded domain. The evaluation is organized around a set of pre-defined properties: accuracy of individual operators, accuracy of the whole scheme, conservation of key quantities, control of the divergence variable, representation of the energy and enstrophy spectra, and simulation of nonlinear dynamics. The results confirm that the scheme is between the first and second order accurate, and conserves the total energy and potential enstrophy up to the time truncation errors. The scheme is capable of producing more physically realistic energy and enstrophy spectra, indicating that it can help prevent the unphysical energy cascade towards the finest resolvable scales. With an optimal representation of the dispersive wave relations, the scheme is able to keep the flow close to being non-divergent, and maintain the geostrophically balanced structures with large-scale geophysical flows over long-term simulations.

Keywords Dispersive wave relations · Energy conservation · Enstrophy conservation · Hamiltonian principles · Shallow water equations · Unstructured meshes

Mathematics Subject Classification 35Q86 · 86-08 · 86-10 · 37K06 · 65P10

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1 Introduction

In long-term simulations of the geophysical flows, where millions of iterations are involved, numerical accuracy alone cannot ensure an accurate representation of certain essential statistics about the flows. Low-order numerical schemes armed with better conservative properties and dispersive wave representations can sometimes reproduce more realistic dynamics than higher order numerical schemes do ([1, 2]). Many authors have been inspired to search for numerical schemes that are not necessarily more accurate, but possess more desirable properties in conservation of key quantities, such as mass, energy, enstrophy, and/or representation of the dispersive wave relations ([13, 17, 19, 32, 33, 44]; see also [23] from a different context). It is in the same spirit that we developed, in a separate article (see [12, called CJT1 hereafter]), a new numerical scheme that conserves both the total energy and potential enstrophy, and possesses the optimal dispersive wave relations on unstructured meshes over bounded or unbounded domains. In tribute to its doubly conservative property (in energy and enstrophy), we call the scheme EEC hereafter. This article is closely related to [12], and its goal is to numerically evaluate the EEC scheme developed there.

A focal question in the evaluations of a new scheme is what advantages it has over conventional numerical schemes that lack some of its properties. More specifically, we would like to understand how the energy and enstrophy conservations, and the representation of the dispersive wave relations affect the long-term dynamics of the simulated flows. To fully address these important questions requires extensive tests using real-world applications, which are out of the reach and scope of the current article, and are left for future endeavors. In this article, we present a preliminary study of these questions in a somewhat idealized setting. For the effect of the energy and enstrophy conservations, Arakawa and Lamb ([2]) make use of an idealized test case with a meridional ridge within a zonal reentrant channel, and show that, a few weeks out into the simulations, their total energy and potential enstrophy conserving scheme, compared with a non-conserving scheme, is better at eliminating the spurious inverse energy cascade, and leads to a less noisy and more organized wind field. Here, we take a similar approach, and perform, among all the tests, a comparative study using an external numerical model, the so-called MPAS-sw model (for the shallow water equations), and an existing test case (the shallow water standard test case #5 with mountain topography). On a global sphere, the MPAS-sw model operates on exactly the same kind of orthogonal meshes as our model does, and therefore it is an ideal choice for comparisons. In this study, we not only examine the vorticity dynamics, but also compute and compare the energy and enstrophy spectra for the two models at different points during the simulations. As for the representation of the dispersive wave relations, it is commonly accepted that it has profound impact on the geostrophic adjustment process ([1, 31]), but we are not aware of any numerical studies of its effect in long-term real applications. In this project, we also perform a second comparative study, comparing our model with the MPAS-sw model in terms of the control of the divergence variable. The rationale for this study is simple: a geostrophically balanced flow should stay close to being non-divergent.

With the focus in mind of the potential impacts of the new scheme in real applications, this numerical study is conducted around the scheme’s properties, rather than around the established test cases, as is usually done in the literature ([8, 13, 33, 43]). Specifically, this study considers six properties of the numerical scheme, which are deemed essential for the success of long-term simulations: the accuracy of the individual operators, the accuracy of the whole model, the conservation of key quantities, the control of the divergence variables, the representation of the energy and enstrophy spectra, and the simulation of the barotropic
instabilities. Each property is evaluated using well selected or specially designed test cases. The rest of the article is organized as follows. Section 2 recalls the conservative numerical scheme that we will investigate. Section 3 presents an iterative procedure for solving the elliptic system that connects the streamfunction and velocity potential with the vorticity and divergence variables. Section 4 presents the numerical results. Finally, some discussions and remarks are provided in Sect. 5.

2 The Conservative Schemes

The numerical schemes are derived in our earlier paper [12, hereafter referred to as CJT1]. In this article we briefly recall those schemes and the main design principles behind them. The goal here is to introduce the schemes so that they can be visually connected to the underlying PDE system.

The vorticity-divergence form of the nonlinear rotating shallow water equations on a two-dimensional manifold \( M \) reads

\[
\begin{aligned}
\frac{\partial}{\partial t} \phi + \nabla \cdot (\phi u) &= 0, \\
\frac{\partial}{\partial t} \zeta + \nabla \cdot (q \phi u) &= 0, \\
\frac{\partial}{\partial t} \gamma - \nabla \times (q \phi u) &= -\Delta (g(\phi + b) + K).
\end{aligned}
\]

Here, \( M \) may be a bounded region on the global sphere, or the entire global sphere. The symbol \( \phi \) stands for the fluid top-to-bottom thickness, \( u \) the horizontal velocity field of the fluid, \( \zeta \equiv \nabla \times u \) the relative vorticity, \( \gamma \equiv \nabla \cdot u \) the divergence. Besides these prognostic variables, the symbol \( q \equiv (f + \zeta)/\phi \), with \( f \) denoting the Coriolis parameter, represents the so-called potential vorticity, \( g \) the gravity constant, and \( K \equiv |u|^2/2 \) the kinetic energy per unit volume. Finally, the bottom topography is given by \( b \).

When treated as a single variable ([35–37]), the mass flux \( \phi u \) possesses a Helmholtz decomposition ([18, 42])

\[
\phi u = \nabla^\perp \psi + \nabla \chi,
\]

where \( \psi \) and \( \chi \) are the streamfunction and the velocity potential respectively, and \( \nabla^\perp = k \times \nabla \) is the skewed gradient operator. In the classical Helmholtz decomposition, \( \psi \) is already assumed to satisfy the homogeneous Dirichlet boundary condition ([18]); to enforce the no-flux boundary condition on the flow, one only needs to set the normal derivative of the velocity potential \( \chi \) to zero on the boundary, and thus the boundary conditions on \( \psi \) and \( \chi \) are

\[
\begin{aligned}
\psi &= 0, & \text{on } \partial M, \\
\frac{\partial \chi}{\partial n} &= 0, & \text{on } \partial M.
\end{aligned}
\]

The relation between \((\psi, \chi)\) and the vorticity and divergence \((\zeta, \gamma)\) can be easily derived,

\[
\begin{aligned}
\nabla \times \left( \phi^{-1} (\nabla^\perp \psi + \nabla \chi) \right) &= \zeta, \\
\nabla \cdot \left( \phi^{-1} (\nabla^\perp \psi + \nabla \chi) \right) &= \gamma.
\end{aligned}
\]
Under the boundary conditions just given in (3) and with a strictly positive thickness field \( \phi \), the system (4) is a coupled, self-adjoint, and strictly elliptic system for \((\psi, \chi)\).

By substituting the mass flux \( \phi u \) (2) into (1), we can eliminate the velocity variable from the shallow water system entirely,

\[
\begin{align*}
\frac{\partial}{\partial t} \phi + \Delta \chi &= 0, \\
\frac{\partial}{\partial t} \zeta + \nabla \cdot (q \nabla \psi) + \nabla \cdot (q \nabla \chi) &= 0, \\
\frac{\partial}{\partial t} \gamma - \nabla \times (q \nabla \psi) - \nabla \times (q \nabla \chi) &= -\Delta (g \phi + b + K).
\end{align*}
\]

(5)

As it turns out, this is the form that the to-be-derived numerical schemes bear close resemblance to.

The inviscid shallow water system (5) ([29, 48]) is a Hamiltonian system ([34]), and can be put in the canonical form,

\[
\frac{\partial}{\partial t} F = \{F, H\}.
\]

(6)

Here, \( F \) represents a functional associated with the shallow water system, and \( H \) the Hamiltonian, which is also a functional and is, for the shallow water system (1), given by

\[
H = \int_\mathcal{M} \left( \frac{1}{2} \phi^{-1} \left( |\nabla \psi|^2 + |\nabla \chi|^2 + 2 \nabla \psi \cdot \nabla \chi \right) + \frac{1}{2} g (\phi + b)^2 \right) dx.
\]

(7)

The Poisson bracket \( \{\cdot, \cdot\} \) has three components,

\[
\{F, H\}_{\zeta \zeta} = \{F, H\}_{\zeta \gamma} + \{F, H\}_{\gamma \gamma} + \{F, H\}_{\phi \zeta \gamma},
\]

(8)

and each component is defined as follows,

\[
\{F, H\}_{\zeta \zeta} = \int_\mathcal{M} q J(F_{\zeta}, H_{\zeta}) dx,
\]

(9a)

\[
\{F, H\}_{\gamma \gamma} = \int_\mathcal{M} q J(F_{\gamma}, H_{\gamma}) dx,
\]

(9b)

\[
\{F, H\}_{\phi \zeta \gamma} = \int_\mathcal{M} \left[ q (\nabla F_{\gamma} \cdot \nabla H_{\zeta} - \nabla H_{\gamma} \cdot \nabla F_{\zeta}) + (\nabla F_{\phi} \cdot \nabla H_{\phi} - \nabla H_{\phi} \cdot \nabla F_{\phi}) \right] dx.
\]

(9c)

In the above, \( F_{\zeta}, \) etc., are short-hands for the functional (Fréchet) derivatives \( \delta F / \delta \zeta, \) etc. The potential vorticity \( q \) is the same as the one that appears in the momentum formulation (1). \( J(\cdot, \cdot) \) is the Jacobian operator, defined as

\[
J(a, b) = \nabla^\perp a \cdot \nabla b
\]

(10)

for any pair of scalar functions \( a \) and \( b \). The Jacobian operator is skew-symmetric w.r.t. its two argument functions.

As a consequence of the skew-symmetry of the Jacobian operator and the permutations present in its third \( \{\phi \zeta \gamma\} \) component, the Poisson bracket (8) is skew-symmetric. Therefore, when \( F \) is replaced by \( H \) in (6), the right-hand side vanishes, implying that the total energy is conserved. It is also easy to check that quantities of the form

\[
C = \int_\mathcal{M} \phi q^k dx,
\]

\( \forall k \geq 0 \)
Fig. 1 Placement of discrete variables on a generic dual mesh

are singularities of the Poisson bracket, and therefore quantities of this form, called Casimirs, such as mass, total vorticity, potential enstrophy, etc., are also conserved in the shallow water system.

The discrete numerical schemes are derived in two phases: the Hamiltonian phase and the Poisson phase. In the Hamiltonian phase, one obtains a discretization of the Hamiltonian $H$, defined in (7), by the discrete Hamiltonian, still denoted as $H$,

$$
H = \int_{\mathcal{M}} \left\{ \phi_{h}^{-1} \left( \left| \nabla_{h}^{\perp} \psi_{h} \right|^2 + \left| \nabla_{h}^{\parallel} \chi_{h} \right|^2 + \nabla_{h}^{\perp} \psi_{h} \cdot \nabla \chi_{h} \right) \right\} d\mathbf{x},
$$

(11)

Here, the subscripted variables, such as $\phi_{h}$, are the discretization of the corresponding continuous variables, such as $\phi$, by the finite volume method. The following notational convention is used: subscripted variables (by $h$, $i$, etc.) are discrete, while un-subscripted variables are continuous; un-accented discrete variables are defined at cell centers, while variables with the sign ^ on the top designate edge-defined variables, and variables with the sign ~ designate vertex-defined variables (see Fig. 1). The symbols $\nabla_{h}$ and $\nabla_{h}^{\perp}$ represent the finite difference approximations of the gradient operator $\nabla$ and the skew-gradient operator $\nabla^{\perp}$, respectively. The details are omitted, but can be found in Appendix B of [12,CJT1]. The factor of $1/2$ in the kinetic energy in (7) has disappeared in the discrete version here due to the fact that only one component is used in the inner product of the vector fields. One also notes that the skew-symmetry of the Jacobian term, $\nabla^{\perp} \psi \cdot \nabla \chi$, is preserved in the approximation considered here, which leads to a symmetric elliptic system later.

In the Poisson phase, one obtains approximations to the Poisson brackets. Just like its continuous counterpart, the discrete Poisson bracket also has three components,

$$
\{F, H\}_{h} = \{F, H\}_{h,\phi\zeta \zeta} + \{F, H\}_{h,\phi\gamma \gamma} + \{F, H\}_{h,\phi\zeta \gamma}.
$$

(12)

Each component is given by

$$
\{F, H\}_{h,\zeta \zeta} = \int_{\mathcal{M}} \widehat{q}_{h} J_{h} \left( \frac{\delta F}{\delta \zeta_{h}}, \frac{\delta H}{\delta \zeta_{h}} \right) d\mathbf{x},
$$

(13)

$$
\{F, H\}_{h,\gamma \gamma} = \int_{\mathcal{M}} \widehat{q}_{h} J_{h} \left( \frac{\delta F}{\delta \gamma_{h}}, \frac{\delta H}{\delta \gamma_{h}} \right) d\mathbf{x},
$$

(14)
\[ \{F, H\}_{h, \varphi, \gamma} \equiv 2 \int_{\mathcal{M}} \hat{q}_h \left( \nabla_h F_{\gamma h} \cdot \nabla_h H_{\gamma h} - \nabla_h H_{\gamma h} \cdot \nabla_h F_{\gamma h} \right) dx + 2 \int_{\mathcal{M}} \left( \nabla_h F_{\gamma h} \cdot \nabla_h H_{\varphi h} - \nabla_h H_{\gamma h} \cdot \nabla_h F_{\varphi h} \right) dx. \]  

(15)

In the above, where \( \hat{q}_h \) is the potential vorticity at cell edges, which is a remapping of the potential vorticity \( q_h \) at cell centers, and \( q_h \) is defined as

\[ q_h = \frac{f + \zeta_h}{\phi_h}. \]  

(16)

The discrete vorticity \( \zeta_h \), divergence \( \gamma_h \), and geopotential \( \Phi_h \) (needed later) are defined as follows,

\[
\begin{align*}
\zeta_h &= \nabla_h \times \left( \hat{\varphi}_h^{-1} \nabla_h \psi_h \right) + \frac{1}{2} \left( \nabla_h \times \left( \hat{\varphi}_h^{-1} \nabla_h \chi_h \right) + \nabla_h \times \left( \hat{\varphi}_h^{-1} \nabla_h \tilde{\chi}_h \right) \right), \\
\gamma_h &= \frac{1}{2} \left( \nabla_h \cdot \left( \hat{\varphi}_h^{-1} \nabla_h \psi_h \right) + \nabla_h \cdot \left( \hat{\varphi}_h^{-1} \nabla_h \tilde{\psi}_h \right) \right) + \nabla_h \cdot \left( \hat{\varphi}_h^{-1} \nabla_h \chi_h \right), \\
\Phi_h &= \hat{\varphi}_h^{-2} \left( |\nabla_h \psi_h|^2 + |\nabla_h \chi_h|^2 + |\nabla_h \tilde{\psi}_h \cdot \nabla_h \chi_h + \nabla_h \psi_h \cdot \nabla_h \tilde{\chi}_h |^2 \right) + g(\phi_h + b_h). 
\end{align*}
\]  

(17)

In (17) and in the rest of this article, the long stretched hats \( \hat{\cdot} \) and tildes \( \tilde{\cdot} \) denote the remaps between cell centers and cell edges, and cell centers and cell corners, respectively. Details of these mappings can be found in Appendix B of [12]. The discrete Jacobian operator \( J_h \) in (13) and (14) is a skewsymmetry-preserving approximation to its continuous counterpart,

\[ J_h(a_h, b_h) \equiv \nabla_h a_h \cdot \nabla_h b_h - \nabla_h b_h \cdot \nabla_h a_h. \]  

(18)

The skew-symmetrization of the Jacobian here is reminiscent of the treatment of the quadratic convection term in the discretization of the Navier-Stokes equations ([40, 41]).

On the global sphere, no boundary conditions are needed, but both the second and last equation of (17) contain redundancy, and the solutions are not unique, because adding constants to any solution will still produce a solution to the system. To ensure uniqueness, one can replace one equation from each set with an equation that sets \( \psi_i \) or \( \chi_i \) to a fixed value at a certain grid point. Here, without loss of generality, we pick the cell \( i = 0 \), and set

\[
\begin{align*}
\psi_0 &= 0, \\
\chi_0 &= 0.
\end{align*}
\]  

(19)

On a bounded domain, the discrete streamfunction satisfies the homogeneous Dirichlet boundary conditions, while the homogeneous Neumann boundary conditions for the velocity potential \( \chi_h \) are only implicitly enforced through the specification of the divergence operator, and the velocity potential is set to zero at cell 0 to ensure the unique solvability of the system. Specifically, the boundary conditions for the coupled elliptic system on a bounded domain are

\[
\begin{align*}
\psi_i &= 0, \quad i \in BC, \\
\chi_0 &= 0.
\end{align*}
\]  

(20)

In the above, \( BC \) is a set of all cells on the boundary (Appendix A, [12]).
With this Poisson bracket (12), a discrete Hamiltonian system can be constructed,

\[ \frac{\partial F}{\partial t} = \{ F, H \}_h. \tag{21} \]

An energy-conserving (EC) numerical scheme can be obtained by sequentially setting \( F \) in the above to \( \phi_i, \zeta_i, \) and \( \gamma_i \). Details of the derivation can be found in [12,CJT1], and here we list the EC scheme for the sake of completeness,

\[
\begin{align*}
\frac{d}{dt} \phi_i &= -[\Delta_h \chi_h]_i, \\
\frac{d}{dt} \zeta_i &= -\frac{1}{2} \left[ \nabla_h \cdot \left( \tilde{q}_h \nabla^\perp_h \psi_h \right) \right]_i + \frac{1}{2} \left[ \nabla_h \cdot \left( \tilde{q}_h \nabla^\perp_h \chi_h \right) \right]_i, \\
\frac{d}{dt} \gamma_i &= \left[ \nabla_h \times \left( \tilde{q}_h \nabla^\perp_h \psi_h \right) \right]_i + \frac{1}{2} \left[ \nabla_h \times \left( \tilde{q}_h \nabla^\perp_h \chi_h \right) \right]_i - \Delta_h [\Phi_h]_i - \frac{1}{4|A_i|} \left( \tilde{q}_{e_1} (\chi_i - \chi_{i_1}) + \tilde{q}_{e_2} (\chi_{i_2} - \chi_i) \right).
\end{align*}
\tag{22}\]

The terms preceded by \( 1/4|A_i| \) in the equation for \( \gamma_i \) only appear for boundary cells, i.e. \( i \in BC \).

This scheme just described is guaranteed to conserve the total energy, thanks to the skew-symmetry of the discrete Poisson bracket (12), but it does not conserve the potential enstrophy. The reason is this quantity, given as

\[ Z = \int_M \phi_h q_h^2 dx, \]

is not a singularity of the discrete Poisson bracket. More specifically, it fails to nullify the first component \( \{ \cdot, \cdot \}_{h \zeta \zeta} \) of the Poisson bracket. To remedy this defect, we follow Salmon ([38]), and replace this component by the trilinear Nambu bracket,

\[
\{ F, H, Z \}_{h, \zeta \zeta} = \frac{1}{3} \left( \int_M \nabla_h \cdot \tilde{F}_\zeta \nabla^\perp \nabla_h H \nabla^\perp \nabla_h F \, dx \right) + \int_M \nabla_h \cdot \tilde{Z}_\zeta \nabla^\perp \nabla_h H \nabla^\perp \nabla_h F \, dx \tag{23}\]

This trilinear discrete bracket is skew-symmetric with respect to any two of its three arguments, and as a consequence, it vanishes when \( F \) is set to \( Z \).

The modified Poisson bracket thus has the form

\[ \{ F, H \}_h = \{ F, H, Z \}_{h, \zeta \zeta} + \{ F, H \}_{h, \zeta \gamma} + \{ F, H \}_{h, \gamma \gamma}. \tag{24} \]

The second and third components remain the same as previously defined in (14) and (15), respectively. An energy and enstrophy conserving (EEC) scheme is thus inferred:
### Table 1 | Discrete differential operators and letter symbols

| Operator   | Name                  | Letter symbol |
|------------|-----------------------|---------------|
| $\nabla_h$ | Cell-to-edge gradient | G             |
| $\nabla^+_h$ | Vertex-to-edge gradient | $G^\#$       |
| $\nabla^\perp_h$ | Cell-to-edge gradient | S             |
| $\nabla^\perp_h$ | Vertex-to-edge gradient | $S^\#$       |
| $\nabla_h \cdot (\cdot)$ | Edge-to-cell divergence | D             |
| $\nabla_h \cdot (\cdot)$ | Edge-to-vertex divergence | $D^\#$       |
| $\nabla_h \times (\cdot)$ | Edge-to-cell curl | C             |
| $\nabla_h \times (\cdot)$ | Edge-to-vertex curl | $C^\#$       |
| $\phi_h^{-1}(\cdot)$ | Edge-to-edge multiplication | H           |
| $\tilde{\cdot}$ | Cell-to-vertex mapping | N             |
| $\tilde{\cdot}$ | Vertex-to-cell mapping | M             |
| $\cdot$ | Scaling by cell areas | A             |

$$
\begin{align*}
\frac{d}{dt} \phi_i &= - [\Delta_h \chi_h]_i, \\
\frac{d}{dt} \xi_i &= - \frac{1}{6} \left[ \nabla_h \cdot \left( \tilde{q}_h \nabla^\perp_h \psi_h - \tilde{\psi}_h \nabla^\perp_h q_h \right) + \nabla_h \cdot \left( \tilde{q}_h \nabla^\perp_h \tilde{\psi}_h - \tilde{\psi}_h \nabla^\perp_h \tilde{q}_h \right) \right]_i \\
&\quad - \frac{1}{3} \left[ \nabla^\perp_h \tilde{\psi}_h \cdot \nabla_h q_h - \nabla^\perp_h \tilde{q}_h \cdot \nabla_h \psi_h \right]_i - [\nabla_h \cdot (\tilde{q}_h \nabla_h \chi_h)]_i, \\
\frac{d}{dt} \gamma_i &= \left[ \nabla_h \times (\tilde{q}_h \nabla^\perp_h \psi_h) \right]_i + \frac{1}{2} \left( \left[ \nabla_h \times (\tilde{q}_h \nabla_h \chi_h) \right]_i + [\nabla_h \times (\tilde{q}_h \nabla_h \tilde{\chi}_h)]_i \right) \\
&\quad - [\Delta_h \Phi_h]_i - \frac{1}{4|A_i|} (\tilde{q}_{e_1} (\chi_i - \chi_{i_1}) + \tilde{q}_{e_2} (\chi_{i_2} - \chi_i)).
\end{align*}
$$

The term preceded by $1/4|A_i|$ in the equation for $\gamma_i$ only appears for boundary cells ($i \in \mathcal{BC}$).

## 3 Solution of The Elliptic System

Whether an explicit or implicit time-stepping scheme is used, the elliptic system contained in (17) will have to be solved at every time step. Thus, an efficient solution of the elliptic system is vital to the success of the model. Here, we present an iterative scheme coupled with the Algebraic Multigrid (AMG) method, which exploits the structure of the coefficient matrix for the benefit of performance of the solver. To illustrate the structure, we first write the discrete elliptic system in the usual matrix-vector form. To avoid introducing more symbols, we call the vector corresponding to the discrete function $\psi_h$ by $\psi_h$, and the vector corresponding to $\phi_h$ by $\phi_h$. We also denote the coefficient matrix corresponding to each of the discrete differential operators each by a letter symbol, as detailed in Table 1.

Replacing the discrete differential operators in the discrete elliptic system (the last two equations of (17)) by their corresponding letter symbols, we can express the system as...
\[
\begin{pmatrix}
CHS & \frac{1}{2}(MC^*HG + CHG^*N) \\
\frac{1}{2}(DHS^*N + MD^*HZ) & DHG
\end{pmatrix}
\begin{pmatrix}
\psi_h \\
\chi_h
\end{pmatrix}
= 
\begin{pmatrix}
\zeta_h \\
\gamma_h
\end{pmatrix}
\] (26)

This system, which is a discretization of the elliptic problem (4), is not symmetric. It can be made symmetric by a scaling by the cell areas. Hence, we multiply each row by the diagonal matrix \( A \) representing the cell areas, and we obtain

\[
\begin{pmatrix}
ACHS & \frac{1}{2}(AMC^*HG + ACHG^*N) \\
\frac{1}{2}(ADHS^*N + AMD^*HS) & ADHG
\end{pmatrix}
\begin{pmatrix}
\psi_h \\
\chi_h
\end{pmatrix}
= 
\begin{pmatrix}
A\zeta_h \\
A\gamma_h
\end{pmatrix}
\] (27)

Due to the symmetry of the whole system, we have that \( ACHS \) and \( ADHG \) are symmetric, and

\((AMC^*HG + ACHG^*N)^T = (ADHS^*N + AMD^*HS)\). (28)

Due to the fact that \( C = D \) and \( G = S \), we actually have

\( ACHS = ADHG \). (29)

In addition, thanks to the fact that \( C^* = -D^* \) and \( G^* = -S^* \), we have

\( AMC^*HG = -AMD^*HS \),
\( ACHG^*N = -ADHS^*N \).

Thus, regarding the off-diagonal blocks of (27), we have

\( AMC^*HG + ACHG^*N = -(ADHS^*N + AMD^*HS) \) . (30)

Combining this relation with (28), we find that

\( (AMC^*HG + ACHG^*N)^T = -(AMC^*HG + ACHG^*N) \), (31)

that is the off-diagonal block itself is skew-symmetric.

We denote

\( P = ACHS \), \( Q = ADHG \),
\( R = \frac{1}{2}(AMC^*HG + ACHG^*N) \),
\( X = \psi_h \), \( Y = \phi_h \),
\( F = A\zeta_h \), \( G = A\gamma_h \).

Taking (30) into account, we can write the linear system (27) succinctly as

\[
\begin{pmatrix}
P & R \\
R^T & Q
\end{pmatrix}
\begin{pmatrix}
X \\
Y
\end{pmatrix}
= 
\begin{pmatrix}
F \\
G
\end{pmatrix}
\] (32)

This system is a straight transcription of the discrete system (17)\textsuperscript{2,3}. The boundary conditions, (19) or (20), can be incorporated into the system by modifying entries of the coefficient matrices \( P \), \( Q \), \( R \), and the right-hand side vectors \( F \) and \( G \). Modifying the entries of the matrices according to the boundary conditions will retain the symmetry of the linear system (32), and render it invertible, and thus uniquely solvable.
For large-scale linear systems, especially those that have to be solved repeatedly, finding a solver that is efficient in memory and scales with the matrix size is essential. Direct solvers, such as the LU factorization, perform poorly on both fronts, because they have to store the factorizations, which may be non-sparse, and they often have a computing load of $O(n^3)$. Krylov-type iterative schemes, e.g. CG, are very efficient on memory, but as the matrix size grows, the convergence slows down dramatically, making them unsuitable for large-sized ($\geq 40,000$) problems. The Geometric Multigrid Method (GMG) performs superbly in terms of both memory and speed, if nested meshes are used and there is an inherent geometric structure in the coefficient matrix. Unfortunately, we use generally unstructured meshes, and such a geometric structure is absent. This leaves the algebraic multigrid method (AMG) our only choice. The performance of the AMG is less robust than that of the GMG, but it has the advantage that it can be used as a black-box solver to any kind of linear systems.

In our experiments, the AMG is applied to the linear system (32). It is observed that the convergence slows down, as manifested by the increase in the number of iterations required, as the matrix size grows. For example, on a small mesh with about 10K grid points (matrix size $\approx 20K \times 20K$), the AMG requires less than 100 iterations to converge, while on a large mesh with about 600K grid points (matrix size $\approx 1.2M \times 1.2M$), the AMG requires over 500 iterations! AMG usually performs well on classical problems, such as the Poisson equation. The system (32) results from the discretization of two coupled Poisson equations. The submatrices $P$ and $Q$ come from discretization of these two Poisson equations, while the off-diagonal block matrices $R$ are the result of the coupling, albeit weak, between these two. Hence, our hypothesis is that the slow-down of the AMG is due to the departure of the coefficient matrix from that of a single Poisson equation, in both the increased size and the non-zero off-diagonal entries.

To remedy the slow-down of the AMG on the coupled system (32), we introduce an iterative scheme, which works with the AMG to solve the system. The main idea of this iterative scheme is that the entries in the off-diagonal matrix $R$ are generally very small (they would vanish completely if the thickness field is uniform), and thus they can be moved to the right-hand side, and be treated as known quantities in an iterative process. To be precise, we assume that, in the iterative process, $X^n$ and $Y^n$ are already known. Then an update of these variables can be found by solving

\begin{align}
P X^{n+1} &= F - R Y^n, \\
Q Y^{n+1} &= G - R^T X^n.
\end{align}

The AMG method can be employed on these equations separately, which amounts to solving a single classical Poisson equation. In our experiments, across a wide range of meshes (with grids points 2,000 $\sim$ 600,000), the scheme (33) converges in about $4 \approx 6$ iterations, and within each iteration, the AMG method takes about 20 iterations. With the iterative scheme (33), we are able to solve the coupled linear system (32) with the AMG method with a computational cost that is approximately linear with respect to the size of the problem.

## 4 Numerical Simulations

In this section we present the numerical simulations of the model. Rather than going through various well-established test cases for the shallow water model, as has usually been done in the literature, here, we focus on a few pre-defined properties of numerical models for large-scale geophysical flows, and examine our model with regard to each of these properties.
Table 2  Discrete differential operators. The symbols $\alpha$ and $\beta$ stand for generic scalar variables, and $\alpha_h$ and $\beta_h$ generic discrete variables defined at cell centers. Other notational conventions described in the previous section apply

| Discrete | Analytic |
|----------|----------|
| $\Delta_h \beta_h$ | $\Delta \beta$ |
| $\nabla_h \cdot (\vec{\alpha}_h \nabla \beta_h)$, | $\nabla \times (\vec{\alpha}_h \nabla \beta_h)$ |
| $\nabla_h \times (\vec{\alpha}_h \nabla \beta_h)$, | $\nabla \times (\vec{\alpha}_h \nabla \beta_h)$ |
| $\nabla_h \cdot (\vec{\beta}_h \nabla \alpha_h)$ | $\nabla \times (\vec{\alpha}_h \nabla \beta_h)$ |
| $\nabla_h \times (\vec{\beta}_h \nabla \alpha_h)$ | $\nabla \times (\vec{\alpha}_h \nabla \beta_h)$ |
| $-2 \nabla_h \beta_h \cdot \nabla \alpha_h$ | $-2 \nabla_h \beta_h \cdot \nabla \alpha_h$ |
| $2 \nabla_h \alpha_h \cdot \nabla \beta_h$ | $2 \nabla_h \alpha_h \cdot \nabla \beta_h$ |

Specifically, we will examine our model with regard to six properties: (1) the accuracy of individual operators in the model; (2) the accuracy of the entire model; (3) the conservation of some physical quantities; (4) the control of the divergence variable; (5) the representation of the energy and enstrophy spectra; (6) the simulation of the barotropic instabilities. We believe that these six properties as a whole are essential for the success of long-term simulations of large-scale geophysical flows.

For this numerical study, a selected set of well-established test cases are used, including the famous shallow water standard test cases (SWSTC) #2 (a steady-state zonal flow) and #5 (zonal flow over a mountain topography) from [47], and the barotropic instability test case from [16]. Following [5], we also use an adapted version of the SWSTC #2 on the northern hemisphere. Finally, we also make use of a new test case of our own ([11]) involving a freely evolving gyre in the northern Atlantic.

An external model, the MPAS-sw model, is used for comparison in the examination of certain numerical properties listed above. The MPAS-sw is a C-grid momentum-based shallow water model. This model operates on the same kind of unstructured meshes as our model does (i.e. spherical centroidal Voronoi tessellations with Delaunay duals), and has a similar convergence rate (presumed for our model at this point), but it is designed to conserve the total energy only, not the potential enstrophy. Therefore, it is expected that both models will have similar performances in certain aspects, but will differ in others. What these differences mean for long-term simulations of geophysical flows is of course an interesting and important question to be investigated in subsequent studies.

For all these numerical simulations, the semi-discrete scheme (25) is advanced by the fourth order Runge Kutta (RK4) method. The RK4 is an explicit time stepping method that has a relatively large stability region. The time step size is empirically determined, and is found to scale linearly with the mesh resolution. Specifically, it is found that the method is still stable with $\Delta t = 1440s$ on the 120km mesh, and $\Delta t = 720s$ on the 60km mesh, and so on so forth.

4.1 Accuracy of Individual Differential Operators

Listed in Table 2 are all the discrete differential operators that appear in either the energy-conserving scheme (22) or in the energy and enstrophy-conserving scheme (25). The analytical differential operators, of which these discrete differential operators are, formally,
approximations of, are also listed in the rightmost column of the table. This table contains four groups of differential operators, as divided by the solid lines. Discrete differential operators on the same row are algebraically, as well as numerically, equivalent, while numerical evidence shows that the operators in the same group are very close in accuracy (see below). There are a total of eight discrete differential operators, contained in the third and fourth groups from the table, approximating the analytical differential operator $\nabla \times (\alpha \nabla \psi)$. The three operators in the third group all have the vertex-to-cell mapping as the last operation, while those in the fourth group have the same mapping, but as the very first operation.

All the operators given in Table 2, except the discrete Laplace operator $\Delta_h$, are combinations of three to four individual discrete operators, e.g. the discrete gradient, the discrete divergence, the cell-to-vertex mapping, and the vertex-to-cell mapping. It is reasonable to expect that these composite operators will remain second-order accurate on a planar centroidal Voronoi mesh with perfect hexagons. However, on a regular centroidal Voronoi mesh which consists of mostly hexagons and a few pentagons, the accuracy will likely be degraded. A rigorous numerical analysis of these operators on unstructured meshes will be carried out elsewhere. Here, we examine the accuracy of these operators numerically.

Due to the prominent roles that the remapping (cell-to-vertex, vertex-to-cell, and edge-to-cell) operators play throughout the schemes, we examine the accuracies of these operators first. The cell-to-edge mapping is not included in this study, because the accuracy of this mapping is well understood to be second-order accurate, due to the fact that every two neighboring cell centers are equi-distant to the common Voronoi edge that separates them. We measure the accuracy of the remapping operators by comparing the remapped values from one location to another with the actual values of a pre-chosen scalar analytic function. Specifically, we use a scalar analytic function with mild variations in both latitude and longitude,

$$\psi = a \cos^3 \theta \sin(4\lambda),$$

where $\theta$ and $\lambda$ stand for the latitude and longitude, respectively, and $a = 6371000\text{m}$ the earth radius. Then accuracy of the cell-to-vertex remapping operator, for example, is then computed as follows,

$$\frac{\| \mathcal{R}_{h,v} \psi - \mathcal{R}_{h,c} \psi \|}{\| \mathcal{R}_{h,v} \psi \|}.$$
Fig. 3 The normalized errors of individual discrete operators, along with the first-order and second-order reference convergence curves (solid black lines). The errors in the $L^2$-norm of all four representative operators converge at a rate between the first and second orders, while the errors in the $L^\infty$-norm do not converge, except that of the representative operator from the third group, which converges at approximately the first order.

In the above, $R_{h,c}$ and $R_{h,v}$ stand for the restriction operators at the cell centers and cell vertices, respectively, and the sign $\tilde{\cdot}$ represents the cell-to-vertex remapping, as in the specification of the schemes.

For this test, we use a series of quasi-uniform spherical centroidal Voronoi tessellations (SCVT) with resolutions ranging from 480 km up to 15 km. The $L^2$ norm and the $L^\infty$ norm of the errors from all three remapping operators are calculated, and plotted in Fig. 2. The $L^2$ norms (left panel) of the errors in the edge-to-cell and vertex-to-cell remapping operators all converge towards zero consistently at the second order, while those of the cell-to-vertex operator converge only at the first order. This degradation in the accuracy of the cell-to-vertex remapping operator is likely due to the fact that it is an upscaling remapping from cells ($\times 1$) to vertices ($\times 2$). The $L^\infty$ errors in all three remapping operators start out similarly as the $L^2$ errors, up to the resolution of 120 km. But, onto higher resolutions, the curves for the vertex-to-cell and edge-to-cell operators start to tilt up, and approach the first-order convergence rate after the 30 km resolution. The curve for the cell-to-vertex operator, which is already at a lower convergence rate, exhibits a slight degradation at the highest resolutions. The degradation in the accuracies of all three operators are likely indicators of irregularities in the mesh at the higher resolutions.

We study the accuracies of these discrete differential operators of Table 2 by measuring their normalized truncation errors. To do so, we take

$$\alpha = 10^{-8} \sin \theta \cos \lambda,$$

$$\beta = a \cos^3 \theta \sin 3\lambda,$$

where, again, $\theta$ and $\lambda$ stand for the latitude and longitude, respectively, and $a$ is the earth radius. The magnitudes of these variables are chosen so that the magnitude of $\alpha$ matches the magnitude of the planetary potential vorticity, while that of $\beta$ matches the magnitude of the streamfunction for large-scale planetary flows. The discrete variables $\alpha_h$ and $\beta_h$ are defined by applying the restriction operator $R_h$ to the analytic variable $\alpha$ and $\beta$, respectively. The normalized truncation error of $\nabla_h \cdot (\tilde{\alpha}_h \nabla_h \beta_h)$, for example, is defined as

$$\frac{\| \nabla_h \cdot (\tilde{\alpha}_h \nabla_h \beta_h) - R_h (\nabla \cdot (\alpha \nabla \beta)) \|}{\| R_h (\nabla \cdot (\alpha \nabla \beta)) \|}.$$
The accuracies of all the discrete operators in Table 2 are studied, using a series of mesh resolutions ranging from 480km to 15km. Numerical results show that the normalized truncation errors for operators in the same group are very close, agreeing up to at least the third digits. For this reason, we only plot the results from the first representative member in each group in Fig. 3. On the left are the normalized \( L^2 \)-errors, and it is seen that the errors from all four representative operators converge at a rate between the first and the second orders, with the representative operator \( \nabla_h \times (\hat{\alpha}_h \nabla_h \beta_h) \) from the third group being the most accurate (at the 2nd order) and the representative operator \( \nabla_h \times (\hat{\alpha}_h \nabla_h \hat{\beta}_h) \) from the fourth the least accurate (at the 1st order). The performances of the operators from the first and second groups are in between these two extremes. The difference in the performances of the third and fourth groups are caused by the application of the remapping operators. The operators in the fourth group all start with the cell-to-vertex mapping, while the operators in the third group all finish with the vertex-to-cell mapping. Both mappings are area weighted, but, as shown in Fig. 2, the vertex-to-cell mapping is more regular, as it is a downscaling mapping from vertices (\( \times 2 \)) to cells (\( \times 1 \)), while the cell-to-vertex mapping is more singular, as it is an upsampling mapping from cells (\( \times 1 \)) to vertices (\( \times 2 \)). The convergences for the operators from all groups are consistent across the whole range of mesh resolutions, except the operator \( \nabla_h \cdot (\hat{\alpha}_h \nabla_h \beta_h) \) at the highest resolution 15km. We suspect that this flat-out is caused by an anomaly in the mesh.

On the right of Fig. 3 are the normalized \( L^\infty \) errors. The \( L^\infty \) errors for most of the operators are not converging, which is expected. It is therefore surprising to see that the \( L^\infty \) errors for the representative operator \( \nabla_h \times (\hat{\alpha}_h \nabla_h \beta_h) \) from the third group actually converge at the first order. This operator also has the best and most consistent \( L^2 \) converging rates.

The above results concerning the individual operators of Table 2, except the third group, largely agree with those of [14, Section 6.2] on the SCVT grids in that the operators are between first and second order accurate in the \( L^2 \) norm, and non-consistent in the \( L^\infty \) norm. In addition to the SCVT, other types of optimized grids are also considered in the work just referenced, and one particular type, the so-called tweaked icosahedra, is shown to lead to consistent operators in both the \( L^2 \) and \( L^\infty \) norms. Operators in the third group on Table 2 are not needed, and hence not studied in [14].

4.2 Accuracy of The Entire Model

4.2.1 A Stationary Zonal Flow on The Global Sphere (SWSTC#2) and on A Hemisphere

The SWSTC #2 specifies an initial zonal flow that is in perfect geostrophic balance. Thus, this test case not only provides a rare means of testing the accuracy of numerical schemes with an analytic solution to the full SWEs, it is also an excellent test on the capability of a numerical scheme to maintain the geostrophic balance. In order to test the impact of the presence of a boundary on the accuracy of the numerical scheme as well as its capability to maintain geostrophic balance, we follow [5] and run the same test, with the same initial conditions, but on the northern hemisphere, with the equator serving as the southern boundary. Both the EC scheme (22) and the EEC scheme (25) are used for this test case, and the results are very similar. Hence we only present and discuss the results from the EEC scheme.

The exact configurations of the SWSTC #2 can be found in the original Williamson et al article ([47]) and many other numerical articles that followed. We run the test for 5 days, as recommended in the original article, on a suite of quasi-uniform meshes on the global sphere, with resolutions ranging from 480km to 30km. Then we compare the solutions on
Fig. 4 SWSTC #2: Convergence in the $L^2$ (left) and $L^\infty$ (right) norms. The errors in the thickness and vorticity variables are relative, while the errors in the divergence variables are the absolute errors, and their $L^2$ norms are area-weighted and -normalized.

day 5 with the initial state, and compute the normalized $L^2$ and $L^\infty$ errors. The same test is then carried out again, on a suite of quasi-uniform meshes on the northern hemisphere.

The results on the global sphere are plotted against the grid resolution in Fig. 4, together with the first- and second-order reference convergence curves. It is seen that the $L^2$ errors for both the thickness and vorticity variables converge at the second order, with the vorticity errors larger but converging more consistently, all the way up to the 30km resolution. Since the flow starts out as non-divergent and the divergence variable as zero, the area-weighted and -normalized absolute (vs. relative) error is used for the divergence variable. The $L^2$ errors for the divergence variable are very small, and stay below $10^{-8}$ for all resolutions. The $L^2$ errors of the divergence variable are not converging as the mesh refines, probably because these errors come from the round-off errors of the discrete model. This point is further corroborated by the fact that the $L^2$ errors do not seem to increase over time either (see Fig. 11, left panel). The relative $L^\infty$ errors of neither the thickness nor the vorticity show any sustained converging trend, and the $L^\infty$ error of the divergence variables shows a steady growing trend, likely due to the anomalies in the mesh geometry at high resolutions. At 30km, the maximum magnitude of the divergence variables reaches about $10^{-7}$.

For comparison, the thickness variable under the extended Z-grid scheme of Eldred [14] on this particular test case converges at approximately the first order in both the $L^2$ and $L^\infty$ norms, on the so-called tweaked icosahedral grids. Under our scheme, the same variable converges slightly faster in the $L^2$ norm on general SCVT grids, but does not converge in the $L^\infty$ norm, which is consistent with the convergence behaviors of the individual operators, and also agrees with the results (Fig. 7) in [33] on the same SCVT grids; see also [7, 30] for an in-depth discussion of the issue. The convergence behavior of the vorticity variable is not discussed in any of the works just referenced.

The result from the hemisphere case are plotted against the grid resolutions in Fig. 5, together with the first- and second-order convergence reference curves. In this case, the relative $L^2$ errors in the thickness converge at an approximately first-order rate. The relative $L^2$ errors for the vorticity variable are larger, but converge faster, at an approximately second-order rate. The $L^\infty$ errors in neither variable converge consistently. As we already pointed out, the flow starts out non-divergent, and the magnitude of the divergence variable can only go up in time. The figure shows that the magnitude in the divergence variable also goes up as the grid refines, again, likely due to the anomalies in mesh geometries at high resolutions and the fact that these errors are simply manifestation of the round-off errors in the model. The
Fig. 5 A stationary flow on the northern hemisphere: convergence in the $L^2$ (left) and $L^\infty$ (right) norms. The errors in the thickness and vorticity variables are relative, while the errors in the divergence variables are area-weighted and -normalized absolute errors.

Fig. 6 Distribution of the errors in the thickness variable for the SWSTC #2 on the 30km global mesh (Left) and the 30km hemispheric mesh (Right). The same color mapping scale is used for both plots; however, the errors on the hemisphere have a much wider range, $[0, 9.8]$.

area-weighted and -normalized $L^2$ and $L^\infty$ errors reach approximately $10^{-7}$ and $5 \times 10^{-6}$, respectively, at the 30km resolution.

Compared with the SWSTC #2 on the global sphere, the errors in the current case are larger by a factor of 2 to 5, across all variables and for both norms, and the convergences are also slower. The downgraded accuracies can be attributed to the presence of boundaries and the downgraded uniformity in the grid resolution. The spherical centroidal Voronoi tessellations on the global sphere are generated using isohedra as starting points, and the resulting meshes are highly uniform, with a ratio of 1.26 between the highest and lowest resolutions, as represented by the cell-to-cell distances. Errors on this class of meshes tend to be highly uniform as well, except near the 10 pentagons on the mesh, where the largest errors tend to cluster (see the left panel of Fig. 6 for plot of the error distribution on a 30km global SCVT mesh). The pentagons on a mostly hexagonal global mesh are inherited from the original isohedron, and are unfortunately inevitable. The spherical centroidal Voronoi tessellations on bounded domains start with a set of prescribed points on the boundary and a set of largely random points in the interior. With iterations, the meshes can achieve a ratio of 2.54 between the highest and lowest resolutions, which qualifies as quasi-uniform meshes.
4.2.2 Zonal Flow Over A Mountain Topography (SWSTC #5)

This classical test case starts with an initially zonal flow similar to that of the SWSTC #2. The flow impinges on a mountain topography centered at latitude $30^\circ$ and longitude $-90^\circ$, and gradually evolves into a turbulent flow around day 25. The exact configurations of this test case, again, can be found in the reference [47], and will not be repeated here. This test case was originally used by Takacs ([39]) to study the conservation of integral invariants by a posteriori methods. Subsequently, this test case was used by many authors to qualitatively study the capability of numerical schemes to simulate the nonlinear dynamics in geophysical flows (see e.g. [13, 24, 33, 46]).

For this study, we again use a suite of quasi-uniform meshes over the global sphere, with resolutions ranging from 480km to 30km. The relative errors in the thickness field on day 15, under both the $L^2$ and the $L^\infty$ norms, are computed by comparing our solutions to the high resolution spectral solution H213 from ([21]). The relative errors are then plotted against the grid resolutions in Fig. 7, along with the reference first- and second-order convergence curves. It is seen that the errors in both norms converge consistently at a rate between the first and second orders. It should be pointed out that the reference solution is computed with diffusion, while our solutions are computed without any diffusion.

4.3 Conservative Properties

It has been proven in [12,CJT1] that the numerical scheme conserves the first order moments, such as the mass and the absolute vorticity, up to the machine errors, and the total energy and enstrophy, which are second-order moments, up to the time truncation errors. These results are confirmed in the numerical study. Here we present the results from two tests. The

![Fig. 7 SWSTC #5: Errors on day 15 with respect to high-resolution spectral (H213) solutions. The EEC scheme is used. The grid resolutions range from 480km to 60km](image-url)
Fig. 8 The initial stream function of a single gyre in the Northern Atlantic Ocean. The value of the streamfunction is represented by the color as well as the contours. The streamfunction is chosen so that it has a constant value along the boundary.

first test is on a bounded domain, and the results from this test illustrate the impact of the time truncation errors in the conservation of the total energy and the potential enstrophy. The second test is on a global sphere, and involves comparison to a third-party model that is designed to conserve the total energy but not the potential enstrophy.

In numerical schemes, the boundary is often a source of errors. Inconsistent treatment of the boundary conditions can even result in unstable simulations. In order to numerically verify the conservative properties of our numerical scheme and examine its treatment of the boundary conditions, we design a test case with a freely evolving gyre in a bounded domain, with no external forcing or diffusion. Physically, both the total energy and the potential enstrophy should be conserved, alongside the mass and total vorticity, and this should also be the case in numerical simulations with schemes that are designed to conserve these quantities.

For the physical domain, we consider one section of the mid-latitude northern Atlantic ocean (Fig. 8). No bathymetry is taken into account, that is, the bottom of the basin is assumed to be flat.

The initial state of the flow is given by

$$\psi(\lambda, \theta) = e^{-d^2} \times (1 - \tanh(20 \times (d - 1.5))),$$

where

$$d = \sqrt{\frac{(\theta - \theta_c)^2}{\Delta \theta^2} + \frac{(\lambda - \lambda_c)^2}{\Delta \lambda^2}},$$

and the parameters $\theta_c = 0.5088$ and $\lambda_c = -1.1$ are the latitude and longitude of the center point of the Atlantic section, $\Delta \theta = 0.08688$, $\Delta \lambda = 0.15$. The tanh function is used to ensure that the initial stream function is flat (with one constant value) near and along the boundary of the domain. A plot of the domain and the stream function are shown in Fig. 8. This stream function produces a circular clockwise velocity field in the middle of the ocean, with the maximum speed of about $0.8$ m/s near the center, which is considered fast for oceanic flows. No external forcing or diffusion is applied, and the flow is required to satisfy the no-flux boundary conditions, and is otherwise left free. The circular pattern will breakdown eventually, because of the irregular shape of the domain and because of the non-uniform Coriolis force.

We cover this bounded domain with a non-uniform 3088-cell SCVT mesh with resolutions ranging from about 20 km to 160 km. The EEC scheme is employed, together with the RK4
Fig. 9 Normalized changes in the total energy and potential enstrophy in a freely evolving gyre: (a) with a 3088-cell SCVT grid and time step size 80s, and (b) with a 3088-cell SCVT grid and time step size 40s. The losses in the total energy and potential enstrophy come down with reduced time step sizes, confirming that the conservations are up to the time truncation errors.

Fig. 10 SWSTC #5: The normalized changes in the total energy and the potential enstrophy in EEC (left) and MPAS (right) models

time stepping scheme, and the simulation is run for one calendar year (360 days). The total energy and potential enstrophy are computed for each day, and these statistics are then plotted against time in Fig. 9. In order to illustrate the impact of the time truncation errors, we run the simulation twice, with two time step sizes, 80s (left) and 40s (right). At the end (day 360) of the first run with the 80s time step size, the system loses $2.5 \times 10^{-5}$ of the total energy and $1.5 \times 10^{-14}$ of the potential enstrophy (Fig. 9 (a)), with the latter almost in the range of roundoff errors for a simulation of this length. At the end of the second run with the 40s time step size, the system loses $3 \times 10^{-6}$ of the total energy, a reduction compared to the first run by a factor of about 8, and it loses about $4 \times 10^{-15}$ of the potential enstrophy, a reduction by a factor of about 4. These results confirm that the EEC numerical scheme conserve the total energy and potential enstrophy up to the time truncation errors, and with reduced time step sizes, the truncation errors do come down.

Our second test involves an initially zonal flow over a mountain topography over the global sphere(SWSTC #5, [47]). The purposes of this test are two folds. First, it seeks to verify the conservative properties of the EEC scheme in different setting (flow over topography in a global domain), and second, it seeks to contrast the results from our EEC scheme with those of the MPAS-sw model, which operates on the same kind of global SCVT meshes, has similar convergence rates, but is not designed to conserve the potential enstrophy. For this test, both models use a global quasi-uniform SCVT mesh with 40962 cells (res. 120km) and
the RK4 time stepping scheme. The simulations are run for 250 days, and the total energy and potential enstrophy are computed for each day, and then plotted against time in Fig. 10. In the EEC scheme (left panel) the flow experiences a weak decay in both the total energy and the potential enstrophy, likely due to the numerical diffusion of the RK4 time stepping scheme. By the end of the simulation, the flow loses about $2 \times 10^{-6}$ of the total energy and about $1.2 \times 10^{-6}$ of the potential enstrophy. In the MPAS-sw model, the evolution curve of the total energy is similar to that of our EEC scheme, but the potential enstrophy increases by about 40% at the end of the simulation. This shows that numerical accuracy alone cannot guarantee the conservation of all dynamical quantities. Our EEC scheme and the MPAS-sw model share a similar convergence rate, but our scheme is far superior in the conservation of the potential enstrophy ($0.00012\%$ vs $40\%$).

It is worth noting that, our EC scheme, while not proven to conserve the potential enstrophy, manages to only accumulate about $0.8\%$ of it (results not plotted here), highlighting the promising prospect of the Hamiltonian approach for numerical scheme design.

### 4.4 Control of The Divergence Variable

Large-scale geophysical flows constantly evolve around an approximate geostrophical balance, i.e. a balance between the Coriolis force and the pressure gradient. Therefore, it is
Fig. 12 Comparison of the magnitude of the divergence variable from the EEC model (left panel) and the MPAS-sw model (right panel). Data are saved once a day from the SWSTC #5 on the 60km global SCVT, for 250 days. Each dot on the figures represents the normalized $L^2$ or $L^\infty$ norm of the divergence variable at the beginning of the day. The orange lines are the linear regressions of the data points, with the slopes of the lines noted.

It is clearly apparent from the plots that the divergence variable remains largely flat for the EEC model, with a slope of $4.047548 \times 10^{-10}$, indicating no noticeable growth. The $L^\infty$ norm is larger, as expected, but remains largely below $1 \times 10^{-5}$. Again, no noticeable and sustained growth is observed; in fact, the linear regression indicates a downward trend, with a slope $= -4.80 \times 10^{-9}$.

We use the SWSTC #5 again in this experiment to study the capability of our model to control the divergence variable. We carry out the experiment first on the 120km global SCVT mesh. On the left panel of Fig. 11, we plot the evolution of the area-normalized $L^2$ norm and the $L^\infty$ norm of the divergence variable, up to day 250. It is seen that the $L^2$ norm of the divergence variable remains largely flat (linear regression curve having a slope $= 2.47 \times 10^{-10}$), exhibiting no noticeable growth. The $L^\infty$ norm is larger, as expected, but remains largely below $1 \times 10^{-5}$. Again, no noticeable and sustained growth is observed; in fact, the linear regression indicates a downward trend, with a slope $= -4.80 \times 10^{-9}$. Crucial for a numerical scheme to maintain this geostrophic balance in order to be able to accurately simulate the dynamics. It has long been recognized that an accurate representation of the dispersive wave relations is crucial for the success in this task, because a proper representation of the dispersive wave relations allows energies to propagate properly across scales rather than unphysically accumulate at one scale, and eventually destroy geostrophic balance ([1, 31]). Besides its excellent conservative properties, the EEC scheme also possesses the optimal dispersive wave relations. How does this last property contribute to its capability to simulate and maintain geostrophically balanced flows? We need an observable indicator. When flows evolve around the geostrophic balance, the flow is close to being, but not exactly, non-divergent. Therefore, the divergence variable may be an indicator of the capability of a numerical scheme to maintain the geostrophic balance. Ideally, the divergence variable should remain small throughout the simulation.

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We use the SWSTC #5 again in this experiment to study the capability of our model to control the divergence variable. We carry out the experiment first on the 120km global SCVT mesh. On the left panel of Fig. 11, we plot the evolution of the area-normalized $L^2$ norm and the $L^\infty$ norm of the divergence variable, up to day 250. It is seen that the $L^2$ norm of the divergence variable remains largely flat (linear regression curve having a slope $= 2.47 \times 10^{-10}$), exhibiting no noticeable growth. The $L^\infty$ norm is larger, as expected, but remains largely below $1 \times 10^{-5}$. Again, no noticeable and sustained growth is observed; in fact, the linear regression indicates a downward trend, with a slope $= -4.80 \times 10^{-9}$.
For comparison, we also plot the results by the MPAS-sw model on the same scale, on the right panel of the figure. MPAS-sw is a C-grid scheme, with decent but less accurate (vs Z-grid) representation of the dispersive wave relations, when the Rossby deformation radius is not fully resolved ([1]). In the plot, the $L^2$ norm of the divergence exhibits a much higher growth rate, with a slope $= 1.20 \times 10^{-9}$ for the linear regression curve. The $L^\infty$ norm of the divergence exhibits an even higher growth rate, with a slope $= 6.92 \times 10^{-9}$. It is clear that, at 120km, the EEC model outperforms the C-grid MPAS-sw model in controlling the divergence variable and maintaining the geostrophic balance in the flows.

We then repeat the experiment on the finer 60km mesh, and plot the results in Fig. 12. In this experiment, the performance of the EEC model are largely in line with its performance on the coarser 120km mesh. The performance of the MPAS-sw model improves notably, with the linear regressions from the $L^2$ and $L^\infty$ data points now exhibiting $4.85 \times 10^{-10}$ and $3.95 \times 10^{-10}$ slopes, respectively. This improvement can probably be attributed to the fact that C-grid representations of the dispersive wave relations improve when the mesh refines, and approach that of the Z-grid scheme when the grid resolution is far below the Rossby deformation radius ([1, 31]). On this 60km mesh, the performances of the EEC and MPAS-sw are close, with the EEC model maintaining a slight edge in both $L^2$ and $L^\infty$ norms.

In long term climate simulations, low to intermediate resolutions ($\geq 100km$) are still frequently used, due to the limitation of computing power. In addition, global climate models have much complex three-dimensional structures, in which the baroclinic Rossby deformation radii are much smaller than that of the single-layer shallow water model, and the representation of the dispersive wave relations by C-grid schemes will be less than ideal. For these reasons, we believe that, in long term climate modeling, the EEC model has advantages over C-grid based models, such as MPAS, in resolving the dispersive wave relations and maintaining the geostrophic balance in the flows.

Lastly, it should be pointed out that water wave is a ubiquitous phenomenon that appears at both micro and planetary scales, and everywhere in between. The current work involves wave phenomena that appear near the large end of the spectrum (wave length $>> 1km$), that are primarily influenced by the gravity and the inertial (rotational) force, and can be adequately modeled by the large-scale rotating shallow water equations. Water waves at much smaller scales (meters or smaller), in applications such as coastal modeling, tsunami, dam breaking, etc, require specialized wave modeling techniques as well as discretization methods. There is a long and profound history of research in this area as well, and interested readers are referred to [3, 6, 15, 26, 27] among others.

4.5 Representation of The Energy and Enstrophy Spectra

Our EEC scheme excels in combining the desirable conservative and dispersive properties into one scheme. Dynamically, what real advantages does this scheme have compared to other numerical schemes that are currently in operation? Answers to this fundamental question can only be sought by applying the scheme to real-world applications. These important questions will be pursued in the future. Here we examine one crucial dynamical aspect of the numerical scheme, namely its representation of the spectra of the kinetic energy (KE) and potential enstrophy (PEns), and the results are compared with those from the MPAS-sw model, to see what advantages, if any, the EEC model have. According to the phenomenological theories of two-dimensional turbulence ([4, 22, 25]), the KE spectrum of a turbulent two-dimensional flow has a slope of $-3$ in the inertial range, while the spectrum of the PEns has a slope of $-1$. These theories and predictions have been largely confirmed by numerical studies; see
Fig. 13 The vorticity fields (top panel) and the energy (lower panel, solid red curve) and enstrophy (lower panel, blue-dashed curve) spectra from the EEC scheme (left column) and the MPAS-sw scheme (right column) on day 50.

While a correct representation of the KE and PEns spectra does not guarantee a faithful simulation of the nonlinear dynamics of turbulent flows, it is a prerequisite. For this study, we again use the SWSTC #5 with a free zonal flow over a mountain topography. We run both EEC and MPAS-sw over the same global quasi-uniform 120km mesh for 250 days, and we examine and plot the vorticity field and the KE and PEns spectra on day 50 and day 250. Figure 13 shows snapshots of the vorticity field on day 50 from the EEC and the MPAS-sw models. Placed below the snapshots are the plots of the KE and PEns spectra at the same instantaneous moment. The vorticity fields from these two models are qualitatively similar, while the vorticity field of the MPAS-sw appears smoother, due to the fact that, in MPAS-sw, the vorticity is natively defined at the vertices, and is mapped to the cell centers for the visualization purpose. For the EEC model, the KE spectrum demonstrates a slope of $-3$ from wave number 10 to 20, while the PEns spectrum demonstrates a slope of $-1$ from wave number 10 to 30, approximately verifying the phenomenological theories. The KE and PEns from the MPAS-sw model exhibit similar trends. For both models, the KE...
and PEns spectra decay quickly after wave number 30, apparently due to the fact that fluid motions still largely concentrate at large scales, and “cascade” is not complete yet.

This completely changes on day 250 (Fig. 14). For the EEC model, the KE spectrum now displays a slope of \(-3\) from wave number 10 up to wave number 40, indicating that a significant portion of the fluid motion has shifted from the large scales to small scales. Due to this shifting, and due to the lack of diffusion, the PEns spectrum is now distorted with the PEns piling up at high wave numbers, and with no discernible part of the curve conforming to the \(-1\) slope. The results from the MPAS-sw are worse. With this model, the KE spectrum is completely distorted with no discernible part conforming to the \(-3\) slope, and so is the PEns spectrum. For the PEns spectrum, not only is the slope \(-1\) gone, the peak density at high wave number is much larger than the peak density of the PEns from the EEC model, which is most likely due to the spurious source of PEns that we saw in the right panel of Fig. 10. Snapshots of the vorticity fields corroborate what the KE and PEns spectra tell us. Both snapshots are noisy, but the one from the EEC model clearly still possesses some large-scale structures, while the one from the MPAS-sw is completely noisy, with no discernible structures.
4.6 Simulation of Barotropic Instabilities

Instabilities, both barotropic and baroclinic, in the ocean and atmosphere are responsible for the transient and diverse weather phenomena. Therefore, in weather forecast, where accuracy is the primary concern, it is vitally important to accurately simulate the instabilities. But instabilities often happen erratically, if not randomly, and accurately simulating the instabilities in the ocean and atmosphere has been a challenge. The one-layer shallow water model, by nature, is not capable of simulating the baroclinic instabilities. Here, we only exam the capability of our model to simulate the barotropic instability. We will use the familiar Galewsky et al barotropic instability test case ([16]). This test case starts with a perfectly balanced fast zonal jet at 45° north. Due to the barotropic instability, this jet will quickly start to wobble, and eventually give rise to a stream of eddies alongside the jet around day 5, in line with the time scale observed in our weather system. The exact setup of this experiment can be found in the original reference ([16]).

As just mentioned, initially, the thickness and zonal velocity field are in a perfect geostrophic balance. A model with unlimited precision can maintain this balance indefinitely. As pointed out in the original article [16], maintaining this balance is trivial for spectral models using spherical harmonics, because, with all the modes initially horizontal, it will be very difficult for non-horizontal modes to grow. This task is, on the other hand, chal-

![Fig. 15](image.png) The vorticity field on day 5 over latitudes from 45° to 90° in the barotropic instability test case, starting from an unperturbed thickness field. The zonal flow structure is decently preserved by a resolution of 60km and up.
lenging for low-order models based on grids that are not aligned with the latitudes, especially unstructured meshes such as ours. In these models, the discretization errors can quickly get into the system, and distort the geostrophic balance. In our first test, we run the test case using the unperturbed thickness field up to day 5, using a sequence of quasi-uniform SCVT meshes, with mesh resolutions ranging from 480km up to 30km. The goals are (i) to see the effect of the discretization errors at various resolutions, as measured by the departure from the exact geostrophic balance, and (ii) to see what resolution is required to maintain a decent geostrophic balance up to day 5. In Fig. 15, we plot the vorticity field on day 5 from the simulations. In the top two panels for 480km and 240km resolutions, the vorticity exhibit a significant departure from the purely zonal flow, with a Rossby wave as wide as 45° in latitude. At 120km (third panel), which is traditionally placed in the mesoscale range, the Rossby wave width is significantly reduced. At 60km (fourth panel), the maintenance of the geostrophic balance and zonal flow structure is decent.

In order to qualitatively compare the dynamics simulated by our model with previous results, we pick the quasi-uniform 30km mesh, as it is shown in the above that the effect of the truncation errors on this mesh on the overall dynamics is minimal. In Fig. 16, we plot the vorticity field on day 6, for both the inviscid and viscous cases, with the perturbed thickness field. In the inviscid case, the instability is obviously more pronounced. In both cases, the results match those of the previous studies ([9, 16, 45]).

Left unexplored in this work is the question of whether, in the inviscid case, the solution actually converges to a regular solution free of singularities (shocks). Common wisdom say that shocks are inevitable in a compressible system, in the absence of diffusions. The shallow water equations are a slightly compressible system, and the Coriolis force is known to have a regularizing effect. It is not clear whether this regularizing effect can help to suppress the emergence of the shocks. No theoretical results exist concerning one way or the other. In [16], the convergence of the solution in the viscous case is established numerically. The issue in the inviscid case was not explored, due to the prohibitive computational costs. Such costs are also beyond our reach at the moment.

Fig. 16 The vorticity fields on day 6 in the barotropic instability test case, with the perturbed initial thickness field, on a quasi-uniform mesh with 655,362 grid cells (approx. res. 30km)
5 Discussion and Conclusions

This overarching goal of this work is to evaluate the newly developed conservative numerical scheme (EEC), so as to preliminarily assess its potentials in real-world applications. To this end, this work focuses on, and is organized around, a set of pre-defined properties such as accuracy and conservation of key quantities. The evaluations make use of a suite of old and new test cases.

With regard to accuracy, the EEC scheme has a convergence rate between the first and second orders, as evidenced in the SWSTC #2 and #5. On bounded domains, the convergence rate is slightly lower, but remains within that range. On the SWSTC #2, our scheme exhibits a slightly faster convergence rate, second vs first, than the extended Z-grid scheme of Eldred ([14]). This could be attributed to the fact that we use the more accurate area-weighted mapping throughout the scheme, while the extended Z-grid scheme uses less accurate remapping operators for the sake of conservations. Both our work and that of Eldred demonstrate that the accuracy of the numerical scheme is sensitive to the mesh quality.

The EEC scheme is proven to conserve the mass and vorticity up to the roundoff errors, and to conserve the total energy and potential enstrophy up to the time truncation errors. These results are confirmed by the numerical experiments conducted in this study, including one on a bounded domain. A more intriguing question is what advantage(s) a comprehensively conservative numerical scheme has in long-term simulations. Arakawa and Lamb ([2]) argue, via a test case with a channel flow over a ridge, that a doubly conservative scheme can prevent unphysical energy cascades towards the finest resolvable scales. Our study, via a different test case and through a different perspective, confirms this point. We showed that, in the SWSTC #5, the EEC scheme, compared with an energy-conserving only scheme (MPAS-sw), can deliver a more structured vorticity field at the end of a long simulation (250 days), with more physically realistic energy and enstrophy spectra.

The EEC scheme studied here has been shown to possess the optimal dispersive wave relations among the second-order accurate numerical schemes ([12]). It is well known that properly represented dispersive wave relations with positive group speeds are essential to the geostrophic adjustment process, through which large-scale geophysical flows evolve among geostrophically balanced structures. Geostrophic balance is hard to verify directly without the expensive reconstruction of the velocity and pressure fields, but geostrophically balanced flows are close to being non-divergent. Therefore, the divergence variable is a natural choice as an indicator of the maintenance of geostrophically balanced structures in the flows. A flow that starts out geostrophically balanced with a small divergence variable should remain so throughout the simulation period. This is what is observed in the SWSTC #5 with the EEC scheme: the divergence variable remains small and exhibits no discernible growth over a period of 250 days. In contrast, the divergence variable from the MPAS-sw model, based on a C-grid scheme with a decent representation of the dispersive wave relations, shows a slight but unmistakable growth over the same period.

Effort has also been made to assess the capability of the scheme to simulate flow dynamics close to those in the real world. Snapshots of the vorticity field from the Galewsky et al test case demonstrate that while the scheme has a low order of accuracy, it is capable of simulating the barotropic instabilities at mid- to high-resolution, even over unstructured meshes. Unfortunately, the potentials of this scheme in real-world applications cannot be fully assessed in its current implementation, due to the limitations posed by the shallow water model, chief among them the lack of vertical variations and convections. Hence, more work remains to be done in terms of development and testing. On the development side, the
scheme needs to be extended and implemented for more complex models that incorporate vertical variations and convections, such as the primitive equations. On the testing side, real-world applications, or well-designed test cases that are closer to the real-world applications, need to be utilized on the numerical scheme. These important undertakings will be reported elsewhere.

In order to be impactful in real-world applications, the model will have to be able to run efficiently. For this study, the model is implemented for a single CPU, with the possible utilization of a high performance GPU. However, we note that there is nothing in this model that prevents or hinders a parallel implementation on heterogeneous computing architectures, which can be expected to multiply the performance of the model. In the current study, the RK4 time stepping scheme with a uniform time step size is used. Further performance boost is expected from adaptive meshing and local time stepping techniques, as demonstrated in [20]. Implementation of the scheme on modern computer architectures, with advanced adaptive time stepping schemes, constitutes another direction of research that will be separately pursued in the future.

Acknowledgements The first author acknowledges helpful discussions with Leo Rebholz on the iterative scheme for the elliptic system.

Funding The second author was supported in part by US Department of Energy grant DE-SC0020270 and US National Science Foundation grant DMS-2109633. The third author was supported in part by the Research Fund of Indiana University.

Availability of data and material This publication only involves simulation data, which can be reproduced by the numerical model.

Code Availability Code of the numerical model is publicly available at https://github.com/qingshanchen/MOP.

Declarations

Conflicts of interest There are no conflicts of interest.

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