Abstract. An energy-conserving and an energy-and-enstrophy conserving numerical schemes are derived, by approximating the Hamiltonian formulation, based on the Poisson brackets and the vorticity-divergence variables, of the inviscid shallow water flows. The conservation of the energy and/or enstrophy stems from skew-symmetry of the Poisson brackets, which is retained in the discrete approximations. These schemes operate on unstructured orthogonal dual meshes, over bounded or unbounded domains, and they are also shown to possess the same optimal dispersive wave relations as those of the Z-grid scheme.

Key word. Unstructured meshes, shallow water equations, large-scale geophysical flows, energy conservation, enstrophy conservation, Hamiltonian structures, Poisson bracket, dispersive wave relations

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1. Introduction. Long-term weather and climate forecasts remain an challenging enterprise. There are many factors contributing to this challenge, and prominently amidst them is the fact that two major components of the weather and climate systems, namely the ocean and atmosphere, are inherently multi-scale, nonlinear, turbulent, and chaotic. For flows of this nature, accurately reproducing their point-wise behaviors over long-period simulations is out of question. But point-wise behaviors are of little interest for long-term weather and climate forecasts; of far more importance are certain aggregated statistics, such as the annual mean precipitation, likelihood of a drought, etc. How to improve the fidelity of weather and climate models in predicting these statistics is a wide open question with no definitive answers in sight yet. But it is not hard to come up with some obviously necessary conditions for these models to be successful. While the ocean and atmosphere are chaotic in nature, they also very predictably possess some characteristic structures that distinguish them from other physical or engineering flows, such as the gravity-induced stratification and the geostrophic balance between the Coriolis force and the horizontal pressure gradient. Models of these flows, for any chance of success, must reliably reproduce these characteristic structures, for, without them, the model lose any relevance to the large-scale geophysical flows, and can not be trusted to convey any reliable statistics about them. The ocean and atmosphere are close to being inviscid in the interior. When the viscosity is ignored, large-scale geophysical flows conserve many quantities, such as the mass, vorticity, energy, etc. It is then reasonable to expect that models of these flows, under the same assumption, should also conserve at least a select set of these quantities. A model with only half of the mass or energy left at the end of a simulation is unlikely a good approximation of the reality.

This work focuses on these two issues of model developments, namely the preser-
viation of the characteristic structures and the conservation of key quantities. On the
first one, only the preservation of the geostrophic balance will be pursued here. The
issue of stratification will be studied in future works.

The Coriolis force, which is a result of the earth rotation, and the horizontal pres-
sure gradient are two dominant terms in the dynamical equations for both the ocean
and atmosphere. The two dominant forces must approximately strike a balance, and
this balance is called the geostrophic balance. Oceanic and atmospheric flows con-
stantly evolve around the geostrophic balance. The process through which geophysical
flows always manage to keep themselves in the vicinity of a perfect geostrophic bal-
ance is called geostrophic adjustment. It was recognized long time ago ([1]) that a key
element of this process is the dispersion of the internal waves. Thus, the capability
of a model to maintain the geostrophic balance is directly related to its representa-
tion of the dispersive wave relations within the flows. Again, it was discovered long
time ago that the placement of discrete variables have an impact on the representa-
tion of discrete wave relations. Arakawa and Lamb ([1]) studied a suite of staggering
techniques, labeled by single letters from A to E, and demonstrated through analy-
sis that each of these techniques provide a different representation of the dispersive
relations. Among these staggering techniques, the so-called C-grid scheme appears
to be the most popular choice, thanks to its decent dispersive wave relations when
the Rossby deformation radius is adequately resolved. Randall ([21]) proposed an
entirely new staggering, actually non-staggering technique, called the Z-grid scheme,
and it is based on the vorticity-divergence formulation of the dynamical equations. It
was shown that the Z-grid scheme possesses the optimal representation of the disper-
sive wave relations among second-order numerical schemes, regardless of whether the
Rossby deformation radius is resolved or not.

The capability of a numerical model to conserve key quantities is severely limited
by its finite dimensionality. An analytical system, with an infinite number of degrees of
freedom, can conserve many, or even infinitely many quantities. A finite-dimensional
discrete system often struggles to conserve more than a few of these quantities. Energy
and enstrophy are two key quantities for large-scale geophysical flows. In the absence
of the diffusion and the external forcing, both energy and enstrophy are conserved
under the analytical system. But conserving both quantities in discrete systems is
not a trivial task. By incorporating conservations as constraints directly into the
derivation process, Arakawa and Lamb ([2, AL81]) obtained a numerical scheme that
conserve both energy and enstrophy for the shallow water equations (SWEs) over
rectangular and spherical meshes. A fourth-order-accurate version of the Arakawa and
Lamb scheme was presented in ([31]). In a series of papers, Salmon ([25, 26, 27, 28])
utilized the Hamiltonian formulation to obtain numerical schemes that conserve both
energy and enstrophy over rectangular meshes. McRae and Cotter ([16, MC]) derived
an energy and enstrophy conserving scheme using the mixed finite element method.
With the mixed finite element method and the Hamiltonian formulation, Eldred and
Randall ([11]) extended the AL81 scheme onto unstructured meshes over the global
sphere, and also obtained a generalization of the Z-grid scheme, which conserves both
energy and enstrophy. Bauer and Cotter ([3]) extended the MC scheme onto bounded
domain, adding the potential vorticity as a prognostic variable on the boundary.

We aim to develop a numerical scheme that conserves both energy and enstrophy,
and possesses good dispersive wave relations. The scheme should be able to operate
over both bonded and unbounded domains, so that it is applicable to both the ocean
and atmosphere. To achieve these goals, we adopt the vorticity-divergence formulation of the dynamical equations, in the hope that the scheme will inherit the optimal dispersive wave relations of the Z-grid scheme of [21]). For the conservations, we adopt the Hamiltonian approach, which has a long history of success in ensuring the conservation of certain key quantities ([12, 34, 13]).

In the Hamiltonian approach, the energy conservation is tied with the skew-symmetry of the Poisson bracket, and the enstrophy conservation is a consequence of the fact that the quantity is a singularity to the Poisson bracket. In the discrete approximations, as it turns out, preserving the skew-symmetry of the Poisson bracket, and thus the energy conservation, is straightforward, but ensuring that the enstrophy remains a singularity to the Poisson bracket is not. To overcome this difficulty, Salmon ([26]) replaces the bilinear Poisson bracket with the trilinear Nambu bracket, which includes the potential enstrophy as a third input parameter, and is skew-symmetric with regard to all of its parameters. This goes well on unbounded domains, since, in the absence of boundaries, the Poisson bracket and the Nambu bracket are equivalent. But they are not over bounded domains. It is discovered in this study that, while they are not equivalent per se, the vorticity-related components of these brackets are actually equivalent even over bounded domains, thanks to the homogeneous Dirichlet boundary conditions commonly prescribed on the streamfunction. Thus, in departure from the common practice in the literature, we replace the vorticity-related component of the Poisson bracket by its Nambu counterpart, and keeps the rest of the Poisson bracket intact.

This project uses unstructured meshes, specifically the centroidal Voronoi tesselations ([7, 9]) for the model development. Traditionally, structured meshes dominate this field ([4, 15, 30]). In recent years, however, unstructured meshes are becoming popular ([19, 29, 22]), for their capability to maintain high qualities across the entire domain, even at very high resolutions, making themselves an appealing option in the age of exascale computing. Another advantage of unstructured meshes is that they can provide an accurate representation of the coastal lines in the case of ocean modeling.

The rest of the article is organized as follows. Section 2 presents a review of the analytic system of the shallow water equations and its Hamiltonian formulation. Section 3 details the derivation, through the Hamiltonian approach, a numerical scheme that conserves energy only, and a numerical scheme that conserves both the energy and the enstrophy. Section 4 deals with the dispersive wave relations of the newly derived schemes. Section 5 concludes with a few remarks.

2. The continuous system and its Hamiltonian formulation. The shallow water equations (SWEs) for large-scale rotating geophysical flows read as

\[
\begin{align*}
\frac{\partial}{\partial t} \phi + \nabla \cdot (\phi \mathbf{u}) &= 0, \\
\frac{\partial}{\partial t} \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + f \mathbf{k} \times \mathbf{u} &= -\nabla (g(\phi + b)),
\end{align*}
\]

(2.1)

where \(\phi\) represents the fluid thickness, \(\mathbf{u}\) the horizontal velocity field of the flow, \(b\) the topography, \(f\) the Coriolis force due to the earth rotation, \(\mathbf{k}\) the unit vector pointing in the local vertical direction, and finally \(g\) the gravitational acceleration. In geoscience, the so-called vector invariant form of the system is often preferred for its
independence from the choice of the coordinate system and it given by

\[
\begin{align*}
\frac{\partial}{\partial t} \phi + \nabla \cdot (\phi \mathbf{u}) &= 0, \\
\frac{\partial}{\partial t} \mathbf{u} + q \mathbf{k} \times (\phi \mathbf{u}) &= -\nabla (g(\phi + b) + K),
\end{align*}
\]

where \( q \equiv (f + \nabla \times \mathbf{u})/\phi \) stands for the potential vorticity, and \( K \equiv |\mathbf{u}|^2/2 \) the kinetic energy of the flow per unit volume.

Taking curl and divergence of the momentum equation of (2.2), one obtains the vorticity-divergence formulation of the SWEs as

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

where \( \zeta \equiv \nabla \times \mathbf{u} \) represents the relative vorticity, and \( \gamma \equiv \nabla \cdot \mathbf{u} \) the divergence. For a two-dimensional model, such as the SWEs, both \( \zeta \) and \( \gamma \) are scalar quantities, and this is one of the reasons that the vorticity-divergence formulation is preferred on unstructured meshes.

Equation (2.3) makes it clear that the relative vorticity \( \zeta \) is not invariant along fluid paths, and thus is not a tracer-like quantity, in contrast to two-dimensional incompressible flows. For the SWEs and geophysical flows in general, that role is played by the potential vorticity \( q \) mentioned in the above, for one can easily derive from the first two equations of (2.3) that

\[
\frac{\partial}{\partial t} q + \mathbf{u} \cdot \nabla q = 0.
\]

The potential vorticity (PV) \( q \) is a key quantity for large-scale geophysical flows ([20]).

We consider the system on a bounded domain \( \mathcal{M} \). The flow is assumed to be inviscid, and obey the no-flux boundary conditions,

\[
\mathbf{u} \cdot \mathbf{n} = 0, \quad \partial \mathcal{M}.
\]

Under the inviscid SWEs, both the energy and the potential enstrophy are conserved. For the energy conservation, one multiplies (2.2) by \( \phi \mathbf{u} \), (2.2)_1 by \( |\mathbf{u}|^2/2 \), and adds the resulting equations to obtain

\[
\frac{\partial}{\partial t} \left( \frac{1}{2} \phi |\mathbf{u}|^2 \right) + \nabla \cdot \left( \frac{1}{2} |\mathbf{u}|^2 \phi \mathbf{u} \right) = -\phi \mathbf{u} \cdot \nabla (g(\phi + b)).
\]

Integrating this equation over the domain \( \mathcal{M} \), and with the no-flux boundary condition (2.5), one derives the kinetic energy budget for the shallow water system (2.2),

\[
\frac{d}{dt} \int_{\mathcal{M}} \frac{1}{2} \phi |\mathbf{u}|^2 d\mathbf{x} = -\int_{\mathcal{M}} \phi \mathbf{u} \cdot \nabla (g(\phi + b)) d\mathbf{x}.
\]

For the potential energy budget, one starts from (2.2)_1,

\[
\frac{\partial}{\partial t} (\phi + b) + \nabla \cdot (\phi \mathbf{u}) = 0.
\]
Multiplying both sides by $g(\phi + b)$, and integrating over $\mathcal{M}$, one obtains

$$
\frac{d}{dt} \int_{\mathcal{M}} \frac{1}{2} g(\phi + b)^2 x = \int_{\mathcal{M}} \phi \mathbf{u} \cdot \nabla (g(\phi + b)) \, dx.
$$

The no-flux boundary condition (2.5) has been used to rewrite the right-hand side into the current form. It is apparent that the terms on the right-hand sides of (2.7) and (2.9), being of the opposite signs, represent the conversion between kinetic and potential energies within the shallow water system. When added together, the right-hand sides of these two equations cancel, and one arrives at

$$
\frac{d}{dt} \int_{\mathcal{M}} \left( \frac{1}{2} \phi |\mathbf{u}|^2 + \frac{1}{2} g(\phi + b)^2 \right) \, dx = 0,
$$

which proves that the total energy of the system, defined as the sum of the kinetic and potential energies, is conserved.

The conservation of the potential enstrophy can be established using the first two equations of (2.3) only. Indeed, these two equations give rise of the transport equation (2.4) for the potential vorticity $q$. Multiplying this equation by $hq$, one has

$$
\frac{\partial}{\partial t} \left( \frac{1}{2} q^2 \right) + \phi \mathbf{u} \cdot \nabla \left( \frac{1}{2} q^2 \right) = 0.
$$

Multiplying (2.3)_1 by $q^2/2$, one gets

$$
\frac{1}{2} q^2 \frac{\partial}{\partial t} \phi + \frac{1}{2} q^2 \nabla \cdot (\phi \mathbf{u}) = 0.
$$

Adding (2.11) and (2.12), and integrating the resulting equation over $\mathcal{M}$, one obtains

$$
\frac{d}{dt} \int_{\mathcal{M}} \frac{1}{2} \phi q^2 \, dx = 0,
$$

which proves that the potential enstrophy is conserved. In fact, following the same procedure and still using only the first two equations of (2.3), one can show that moments of the PV $q$ of arbitrary orders are conserved, that is,

$$
\frac{d}{dt} \int_{\mathcal{M}} \frac{1}{2} \phi q^k \, dx = 0, \quad \forall \ k \geq 0.
$$

It has been shown in [24] that the inviscid shallow water equations conform to the variational principles of the Hamiltonian mechanics. Furthermore, the system can also be written as the Hamiltonian canonical equations, and the energy conservation then naturally follows from the skew-symmetry of the Poisson bracket, and the potential enstrophy is only one of the countlessly many singularities (or Casimirs) of the bracket, and thus is conserved. Here, we present the Hamiltonian formulation of the SWEs, which will serve as a tour-guide to the development of the numerical schemes in the next section.

We define the Hamiltonian for the SWEs as

$$
H \equiv \int_{\mathcal{M}} \left( \frac{1}{2} \phi |\mathbf{u}|^2 + \frac{1}{2} g(\phi + b)^2 \right) \, dx.
$$
It is not a coincidence that the Hamiltonian is also the total energy of the shallow water system (c.f. (2.10)). In this work, we use $\delta$ to denote the variation of a functional. It is then easy to see that, for the momentum variables,

$$
\delta H = \int_M \left( \phi u \cdot \delta u + \left( \frac{1}{2} |u|^2 + g(\phi + b) \right) \delta \phi \right) \, dx.
$$

(2.16)

Thus, we obtain the following functional derivatives of the Hamiltonian $H$ with respect to the thickness and the momentum,

$$
\frac{\delta H}{\delta \phi} = \frac{1}{2} |u|^2 + g(\phi + b) \equiv \Phi,
$$

(2.17a)

$$
\frac{\delta H}{\delta u} = \phi u.
$$

(2.17b)

We note that the right-hand side of (2.17a), usually called the geopotential, also appears in the vector-invariant form (2.2) and the vorticity-divergence form (2.3) of the shallow water equations. This term will be denoted as $\Phi$ in the sequel.

Salmon has demonstrated in [25, 26, 27] that it is advantageous to use the mass flux $\phi u$ instead of the velocity $u$ itself as diagnostic variables, because this choice allows one to write the kinetic energy, which is a cubic polynomial of $\phi$ and $u$, in a binary form that involves $\phi u$ and $u$,

$$
H = \int_M \left( \frac{1}{2} \phi u \cdot u + \frac{1}{2} g(\phi + b)^2 \right) \, dx.
$$

(2.18)

When treated as a single variable, the mass flux $\phi u$ has a Helmholtz decomposition ([14])

$$
\phi u = \nabla^\perp \psi + \nabla \chi,
$$

(2.19)

where $\psi$ and $\chi$ are the streamfunction and the velocity potential respectively, and $\nabla^\perp = k \times \nabla$. In the classical Helmholtz decomposition, $\psi$ is already assumed to satisfy the homogeneous Dirichlet boundary condition ([14]); to enforce no-flux boundary condition (2.5) on the flow, it only remains for the normal derivative of the velocity potential $\chi$ to vanish on the boundary, and thus the boundary conditions on $\psi$ and $\chi$ are

$$
\psi = 0, \quad \text{on } \partial M,
$$

(2.20a)

$$
\frac{\partial \chi}{\partial n} = 0, \quad \text{on } \partial M.
$$

(2.20b)

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

$$
\begin{cases}
\nabla \times (\phi^{-1}(\nabla^\perp \psi + \nabla \chi)) = \zeta, \\
\nabla \cdot (\phi^{-1}(\nabla^\perp \psi + \nabla \chi)) = \gamma.
\end{cases}
$$

(2.21)

Under the boundary conditions just given in (2.20) and with a strictly positive thickness field $\phi$, the system (2.21) is a coupled, self-adjoint, and strictly elliptic system for ($\psi$, $\chi$).
In terms of the thickness, streamfunction and velocity potential, the Hamiltonian (2.15) can be expressed as

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

Substituting the expression (2.19) into (2.16), we have

\[
\delta H = \int_{\mathcal{M}} (\nabla^\perp \psi \cdot \delta u + \nabla \chi \cdot \delta u + \Phi \delta \phi) dx.
\]

The geopotential \( \Phi \) has been defined in (2.17a). By integration by parts on the right-hand side, one can transfer the differential operators onto the velocity field to produce the vorticity and divergence variables, and rewrite the equation as

\[
\delta H = \int_{\mathcal{M}} (-\psi \delta \zeta - \chi \delta \gamma + \Phi \delta \phi) dx.
\]

The process goes through thanks to the boundary conditions (2.5) and (2.20), and the fact that differential operators (\( \nabla^\perp \) and \( \nabla \)) and the variation operator \( \delta \) are inter-changeable.

From the relation (2.24), one easily derive the functional derivatives of \( H \) with respect to the thickness \( \phi \), vorticity \( \zeta \) and divergence \( \gamma \),

\[
\frac{\delta H}{\delta \phi} = \Phi, \quad \frac{\delta H}{\delta \zeta} = -\psi, \quad \frac{\delta H}{\delta \gamma} = -\chi.
\]

With the aid of the Poisson bracket [25], the system (2.3) can be put in the canonical form

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

Here, \( F \) represents a functional associated with the shallow water system, and \( H \) the Hamiltonian, which is also a functional. The Poisson bracket \( \{ \cdot, \cdot \} \) has three components,

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

and each component is defined as follows,

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

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

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

In the above, \( F_\zeta, \) etc., are short-hands for the functional derivatives \( \delta F/\delta \zeta, \) etc. The potential vorticity \( q \) for the SWEs is given by

\[
q = \frac{f + \zeta}{\phi},
\]
and $J(\cdot, \cdot)$ is the Jacobian operator defined by

$$(2.30) \quad J(a, b) = \nabla^\perp a \cdot \nabla b$$

for any two functions $a$ and $b$. The Jacobian operator is skew-symmetric w.r.t. its two argument functions.

A state function, such as the vorticity $\zeta(x, t)$, can be viewed as a parametric functional, and can be cast into the functional form using the parametric Kronner delta function, e.g.

$$F(x, t) \equiv \zeta(x, t) = \int_M \delta(x, y)\zeta(x, t)dy, \quad \forall x \in M, t > 0.$$  

By setting the functional $F$ to $\phi$, $\zeta$, and $\gamma$ in (2.27), one recovers the evolution equation (2.3)\textsubscript{1}, (2.3)\textsubscript{2}, and (2.3)\textsubscript{3}, respectively. Thus, all the prognostic variables, the fluid thickness $\phi$, vorticity $\zeta$, and divergence $\gamma$ evolve according to the differential equation (2.26).

A crucial implication of the Hamiltonian approach is that an arbitrary functional of these state variables, $F = F(\phi, \zeta, \gamma)$ also evolves according to this equation.

**Theorem 2.1.** An arbitrary functional $F = F(\phi, \zeta, \gamma)$ of the state variables also evolves according to the equation (2.26).

To see this, one takes the variation of this quantity, and divides it by a variation in time $\delta t$ to obtain

$$\delta F = \int_M \left( \frac{\delta F}{\delta \phi} \delta \phi + \frac{\delta F}{\delta \zeta} \delta \zeta + \frac{\delta F}{\delta \gamma} \delta \gamma \right) dx,$$

$$\frac{dF}{dt} = \int_M \left( \frac{\delta F}{\delta \phi} \frac{\partial \phi}{\partial t} + \frac{\delta F}{\delta \zeta} \frac{\partial \zeta}{\partial t} + \frac{\delta F}{\delta \gamma} \frac{\partial \gamma}{\partial t} \right) dt.$$

Each state variable evolves according to equation (2.26). Thus one can replace the time derivatives on the right-hand side by the corresponding Poisson brackets,

$$\frac{dF}{dt} = \int_M \left( \frac{\delta F}{\delta \phi} \{\phi, H\} + \frac{\delta F}{\delta \zeta} \{\zeta, H\} + \frac{\delta F}{\delta \gamma} \{\gamma, H\} \right) dt.$$

The next steps in this demonstration is to replace the Poisson brackets by their explicit forms given in (2.27) and (2.28), switch the order of integration, and show that the right-hand side of the equation above equals $\{F, H\}$. Thus the equation (2.26) holds for an arbitrary functional $F$ of the state variables.

It is clear that the Poisson bracket (2.27) is skew-symmetric with respect to its two arguments, and thus

$$\{H, H\} = 0,$$

and

$$(2.31) \quad \frac{d}{dt} H = 0.$$  

The Hamiltonian for the shallow water system, which also identifies with the total energy, is automatically conserved, thanks to the skew-symmetry of the Poisson bracket.
Let $G(s)$ be an arbitrary function of its scalar argument. We now show that a quantity in the form of

$$C = \int_{\mathcal{M}} \phi G(q) d\mathbf{x}$$

is a Casimir of the Poisson bracket. We first notice that

$$\delta C = \int_{\mathcal{M}} (G(q) - q G'(q)) \delta \phi + G'(q) \delta \zeta.$$

Thus, one has

$$\frac{\delta C}{\delta \phi} = G(q) - q G'(q), \quad \frac{\delta C}{\delta \zeta} = G'(q), \quad \frac{\delta C}{\delta \gamma} = 0.$$

Let $A$ be an arbitrary functional. After some algebraic operations, one finds that

$$\{C, A\} = \int_{\mathcal{M}} \nabla C \phi \cdot \nabla \perp A \zeta d\mathbf{x}.$$

As before, $C_\phi$ and $A_\zeta$ are short-hands for the functional derivatives. We assume that the quantity $A_\zeta$ satisfies the boundary condition that

$$\nabla \perp A_\zeta \cdot n = 0, \quad \partial \mathcal{M}.$$

Then we have

$$\{C, A\} = \int_{\partial \mathcal{M}} C_\phi \nabla \perp A_\zeta \cdot n ds = 0.$$

We thus have shown that

$$\{C, A\} = 0, \quad \forall \ A \text{ satisfying (2.36)}.$$

The Hamiltonian $H$ clearly satisfies the condition (2.36). As a direct consequence of (2.37), an infinite number of quantities, in the form of $C$ of (2.32), are conserved under the shallow water system. In particular, the mass (with $G(q) = 1$), total circulation (with $G(q) = q$), and potential enstrophy (with $G(q) = q^2/2$) of the system are conserved.

3. Specification of the schemes. The goal is to develop numerical schemes that conserve energy and/or (potential) enstrophy over arbitrary bounded domains. Our approach is to use the Hamiltonian formulation. We use an unstructured and orthogonal dual mesh, in which the dual cell edges are perpendicular to the associated primal cell edges. A typical example is the Delaunay-Voronoi dual mesh. Detailed specifications of the meshes are given in Appendix A. Specifications of discrete variables and discrete differential operators on these meshes are listed in Appendix B. Finally, a discrete vector calculus, including many of the identities and formulas that will be frequently used in the sequel, is presented in Appendix C.

The focus will be on the symmetry of the Poisson brackets. Per discussions from the previous section, (skew-)symmetries will naturally lead to conservative properties that are desirable for numerical simulations of large-scale geophysical flows. The canonical equations for the fluids contain essentially two ingredients: the Hamiltonian
and the Poisson bracket. Thus, a numerical discretization of the fluid system, based on the Hamiltonian formulation, naturally comprises two phases: the Hamiltonian phase approximating the Hamiltonian, and the Poisson phase approximating the Poisson bracket. It will become apparent later that these two phases are independent of each other.

### 3.1. The Hamiltonian phase

We enter the Poisson phase first. The results from this phase are common to all the schemes that will be presented later.

As a vorticity-divergence based system, the prognostic variables are thickness $\phi_h$, vorticity $\zeta_h$, and divergence $\gamma_h$ at the (primary) cell centers. One will also need the following diagnostic variables: the geopotential $\Phi_h$, the streamfunction $\psi_h$, and the velocity potential $\chi_h$. The current work adopts the convention that subscripted variables (by $h$, $i$, etc.) are discrete, while un-subscripted variables are continuous; un-accented discrete variables are defined at cell centers, while $^\sim$ on the top designates edge-defined variables, and $^\tau$ designates vertex-defined variables.

One approximates the Hamiltonian, defined in (2.22), by the discrete Hamiltonian, still denoted as $H$,

$$
H = \int_M \left\{ \frac{1}{\phi_h^2} \left( |\nabla_h^\perp \psi_h|^2 + |\nabla_h \chi_h|^2 + \nabla_h^\perp \psi_h \cdot \nabla_h \chi_h + \nabla_h^\perp \psi_h \cdot \nabla_h \chi_h \right) + \frac{1}{2} g(\phi_h + b_h)^2 \right\} d\mathbf{x}.
$$

The factor of 1/2 in the kinetic energy in (2.22) 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 is preserved in the approximation here, which leads to a symmetric elliptic system later.

We now derive formulas for the discrete geopotential, vorticity, and divergence. These formulas will connect the diagnostic variables $\psi_h$ and $\chi_h$ to the prognostic variables $\phi_h$, $\zeta_h$, and $\gamma_h$ of the system. We begin by writing down the variation of $H$ defined in (3.1),

$$
\delta H = \int_M \left\{ -\phi_h^{-2} \left( |\nabla_h^\perp \psi_h|^2 + |\nabla_h \chi_h|^2 + \nabla_h^\perp \psi_h \cdot \nabla_h \chi_h + \nabla_h^\perp \psi_h \cdot \nabla_h \chi_h \right) \delta \phi_h \\
+ \phi_h^{-1} \left( 2\nabla_h^\perp \psi_h \cdot \delta \nabla_h \chi_h + 2\nabla_h \chi_h \cdot \delta \nabla_h \psi_h \\
+ \nabla_h^\perp \psi_h \cdot \delta \nabla_h \chi_h + \nabla_h \chi_h \cdot \delta \nabla_h^\perp \psi_h + \nabla_h^\perp \psi_h \cdot \delta \nabla_h \chi_h + \nabla_h \chi_h \cdot \delta \nabla_h^\perp \psi_h \right) \\
+ g(\phi_h + b_h) \delta \phi_h \right\} d\mathbf{x}.
$$

The sign of the first term inside the integral is not right for the geopotential. Switching the sign of the first term, and combining the difference with the terms in the middle, one can write $\delta H$ as

$$
\delta H = \int_M \left\{ \phi_h^{-2} \left( |\nabla_h^\perp \psi_h|^2 + |\nabla_h \chi_h|^2 + \nabla_h^\perp \psi_h \cdot \nabla_h \chi_h + \nabla_h^\perp \psi_h \cdot \nabla_h \chi_h \right) \delta \phi_h \\
+ g(\phi_h + b_h) \delta \phi_h \\
+ 2\nabla_h^\perp \psi_h \cdot \delta \left( \phi_h^{-1} \nabla_h^\perp \psi_h \right) + 2\nabla_h \chi_h \cdot \delta \left( \phi_h^{-1} \nabla_h \chi_h \right) + \nabla_h^\perp \psi_h \cdot \delta \left( \phi_h^{-1} \nabla_h \chi_h \right) \\
+ \nabla_h \chi_h \cdot \delta \left( \phi_h^{-1} \nabla_h^\perp \psi_h \right) + \nabla_h^\perp \psi_h \cdot \delta \left( \phi_h^{-1} \nabla_h \chi_h \right) + \nabla_h \chi_h \cdot \delta \left( \phi_h^{-1} \nabla_h^\perp \psi_h \right) \right\} d\mathbf{x}.
$$
With an application of the adjoint identity (C.1), the terms in the first two lines can be combined together. The discrete integration by parts formulas (C.3), (C.4), (C.7), and (C.8), and the adjoint identity (C.2) are applied to the remaining terms, transferring the differential operators and the remapping operators from the first components of the inner products to the second components. After regrouping these terms based on their associations with the streamfunction $\psi_h$ or the velocity potential $\chi_h$, one obtains

$$\delta H = \int_{\mathcal{M}} \left\{ \left( \delta_h^{-2} \left( |\nabla_h^\bot \psi_h|^2 + |\nabla_h \chi_h|^2 + \nabla^\bot \tilde{\psi}_h \cdot \nabla \chi_h + \nabla^\bot \psi_h \cdot \nabla \tilde{\chi}_h \right) \right) 
+ g(\phi_h + b_h) \delta \phi_h 
- \psi_h \delta \left( \nabla_h \times \left( \tilde{\phi}_h^{-1} \nabla^\bot \psi_h \right) \right) + \frac{1}{2} \left( \nabla_h \times \left( \tilde{\phi}_h^{-1} \nabla \chi_h \right) \right) 
- \chi_h \delta \left( \nabla_h \cdot \left( \tilde{\phi}_h^{-1} \nabla \psi_h \right) \right) + \frac{1}{2} \left( \nabla_h \cdot \left( \tilde{\phi}_h^{-1} \nabla^\bot \psi_h \right) \right) \} \, d\mathbf{x}$$

We set

$$(3.2) \begin{aligned} 
\Phi_h &= \tilde{\phi}_h^{-2} \left( |\nabla_h^\bot \psi_h|^2 + |\nabla_h \chi_h|^2 + \nabla^\bot \tilde{\psi}_h \cdot \nabla \chi_h + \nabla^\bot \psi_h \cdot \nabla \tilde{\chi}_h \right) + g(\phi_h + b_h), \\
\zeta_h &= \nabla_h \times \left( \tilde{\phi}_h^{-1} \nabla^\bot \psi_h \right) + \frac{1}{2} \left( \nabla_h \times \left( \tilde{\phi}_h^{-1} \nabla \chi_h \right) \right) + \nabla_h \times \left( \tilde{\phi}_h^{-1} \nabla \tilde{\chi}_h \right), \\
\gamma_h &= \frac{1}{2} \left( \nabla_h \cdot \left( \tilde{\phi}_h^{-1} \nabla^\bot \psi_h \right) \right) + \nabla_h \cdot \left( \tilde{\phi}_h^{-1} \nabla \psi_h \right) + \nabla_h \cdot \left( \tilde{\phi}_h^{-1} \nabla \chi_h \right). 
\end{aligned}$$

Then the variation of the discrete Hamiltonian $H$ can be written as

$$(3.3) \delta H = \int_{\mathcal{M}} (\Phi_h \delta \phi_h - \psi_h \delta \zeta_h - \chi_h \delta \gamma_h) \, d\mathbf{x}.$$  
This relation leads to the discrete analogues of the functional derivatives given in (2.25),

$$(3.4) \frac{\delta H}{\delta \phi_h} = \Phi_h, \quad \frac{\delta H}{\delta \zeta_h} = -\psi_h, \quad \frac{\delta H}{\delta \gamma_h} = -\chi_h. $$

When the thickness $\phi_h$, the vorticity $\zeta_h$, and the divergence $\gamma_h$ are known, the streamfunction $\psi_h$ and the velocity potential $\chi_h$ can be recovered from the coupled elliptic system (last two equations of (3.2) under proper boundary conditions). On a global sphere, no boundary conditions are needed, but both the second and last equation of (3.2) contains redundancy, and the solutions are not unique, for any solution plus some constants will still be a solution to the system. To ensure uniqueness, one can replace one equation from each set with an equation that sets $\psi_h$ or $\chi_h$ to a fixed value at a certain grid point. Here, without loss of generality, we pick cell $i = 0$, and set

$$(3.5) \begin{aligned} 
\psi_0 &= 0, \\
\chi_0 &= 0. 
\end{aligned}$$

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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 unique solvability of the system. Specifically, the boundary conditions for the coupled elliptic system on a bounded domains are

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

We note that the relations in (3.2) governing the diagnostic variables $(\psi_h, \chi_h)$ and the prognostic variables $(\zeta_h, \gamma_h)$, given a discrete thickness field $\hat{\phi}_h$, are solely determined by the choice of the discrete Hamiltonian $H$. Other choices are certainly possible; but the particularly choice given in (3.1) avoids extra remapping between cell centers and cell vertices, and therefore are more accurate. The skew-symmetry-preserving approximation to the Jacobian term in (3.1) also ensures that the linear operator on the right-hand side of (3.2) is self-adjoint. To see this, we denote the linear operator as $A_h$, given a strictly positive but arbitrary thickness field $\hat{\phi}_h$, and let $(\psi_h^1, \chi_h^1)$ and $(\psi_h^2, \chi_h^2)$ be two sets of diagnostic variables. Then, utilizing the duality identities (C.1), (C.2) about the remappings and the discrete integration by parts formulas (C.3) and (C.4), we find that

\[
\begin{align*}
(A_h \left( \psi_h^1, \chi_h^1 \right)^T, \left( \psi_h^2, \chi_h^2 \right)^T) &= \left( \nabla_h \times \left( \hat{\phi}_h^{-1} \nabla_h \psi_h^1 \right) + \frac{1}{2} \left( \nabla_h \times \left( \hat{\phi}_h^{-1} \nabla_h \chi_h^1 \right) + \nabla_h \times \left( \hat{\phi}_h^{-1} \nabla_h \chi_h^1 \right) \right), \psi_h^2 \right) + \\
&\quad \left( \frac{1}{2} \left( \nabla_h \cdot \left( \hat{\phi}_h^{-1} \nabla_h \psi_h^1 \right) + \nabla_h \cdot \left( \hat{\phi}_h^{-1} \nabla_h \psi_h^1 \right) \right) + \nabla_h \cdot \left( \hat{\phi}_h^{-1} \nabla_h \chi_h^1 \right), \chi_h^2 \right),
\end{align*}
\]

\[
\begin{align*}
&= -2 \left( \hat{\phi}_h^{-1} \nabla_h \psi_h^1, \nabla_h \chi_h^1 \right) - \left( \hat{\phi}_h^{-1} \nabla_h \chi_h^1, \nabla_h \psi_h^2 \right) - \left( \hat{\phi}_h^{-1} \nabla_h \chi_h^1, \nabla_h \psi_h^2 \right) \\
&\quad - \left( \hat{\phi}_h^{-1} \nabla_h \psi_h^1, \nabla_h \chi_h^1 \right) - \left( \hat{\phi}_h^{-1} \nabla_h \psi_h^1, \nabla_h \chi_h^1 \right) - 2 \left( \hat{\phi}_h^{-1} \nabla_h \chi_h^1, \nabla_h \chi_h^2 \right) \\
&= \left( \psi_h^1, \nabla_h \times \left( \hat{\phi}_h^{-1} \nabla_h \psi_h^2 \right) + \frac{1}{2} \left( \nabla_h \times \left( \hat{\phi}_h^{-1} \nabla_h \chi_h^2 \right) + \nabla_h \times \left( \hat{\phi}_h^{-1} \nabla_h \chi_h^2 \right) \right) \right) + \\
&\quad \left( \chi_h^1, \frac{1}{2} \left( \nabla_h \cdot \left( \hat{\phi}_h^{-1} \nabla_h \psi_h^2 \right) + \nabla_h \cdot \left( \hat{\phi}_h^{-1} \nabla_h \psi_h^2 \right) \right) + \nabla_h \cdot \left( \hat{\phi}_h^{-1} \nabla_h \chi_h^2 \right) \right) \\
&= \left( \psi_h^1, \chi_h^1 \right)^T, A_h \left( \psi_h^2, \chi_h^2 \right)^T.
\end{align*}
\]

This shows that the operator $A_h$ is self-adjoint. The main disadvantage of this choice of discrete Hamiltonian is that it is not known under what conditions the linear operator $A_h$ will be (negative) definite. Under normal circumstances, e.g. mild variations in the thickness field, the strictly elliptic terms (second term in (3.2) dominate, and the operator $A_h$ is indeed negative definite. But a precise characterization of the condition for the (negative) definiteness of the operator $A_h$ is not known at this point.

The next two sections deal with the Poisson phase, i.e. discretization of the Poisson bracket. Many approximations exist, each with different properties. We shall
present two approximations. The first approximation preserves the skew-symmetry of the Poisson brackets, and thus leading to a numerical scheme that attains the energy-conserving property of the continuous system. However, the enstrophy is not conserved within this scheme. The second approximation leads to a scheme that conserves both energy and enstrophy.

3.2. The Poisson phase and an energy conserving scheme. In this subsection we present an approximation of the Poisson bracket (2.27) that is skew-symmetric to its two argument. We then derive from this approximation an energy-conserving numerical scheme for the shallow water equations.

The Poisson bracket (2.27) is skew-symmetric w.r.t. \( F \) and \( H \), because each of its three components, defined in (2.28), is skew-symmetric. The first two components (2.28a) and (2.28b) inherits its skew-symmetry from the Jacobian operator \( J(\cdot, \cdot) \). The third component (2.28c) is skew-symmetric due to the inherent permutation in \( F \) and \( H \) within the specification. Thus, the approximations of \( \{ F, H \}_\zeta \zeta \) and \( \{ F, H \}_\gamma \gamma \) will be skew-symmetric if the approximation of the Jacobian operator is so, while an approximation of \( \{ F, H \}_\phi \gamma \) will be skew-symmetric if it retains the inherent permutation of the corresponding discrete variables.

The Jacobian, defined in (2.30), is an inner product of a gradient vector and a skew-gradient vector. A direct approximation of the inner product, e.g. by the finite difference method, will not be skew-symmetric, because the approximation will inevitably involve discrete quantities defined at different locations on the mesh. However, we note that, due to its skew-symmetry, the Jacobian can also be written as

\[
J(a, b) = \frac{1}{2} \nabla^\perp a \cdot \nabla b - \frac{1}{2} \nabla^\perp b \cdot \nabla a.
\]

This new expression for the Jacobian contains a permutation of its two arguments. If this expression is adopted, then no matter how the inner product of the skew-gradient and gradient vectors are approximated, the approximation will be skew-symmetric as long as it retains the permutation of the corresponding discrete variables. With \( a_h \) and \( b_h \) being the discretizations of the analytical functions \( a \) and \( b \), respectively, we write down an approximation of the Jacobian of (3.7),

\[
J_h(a_h, b_h) \equiv \nabla^\perp h \tilde{a}_h \cdot \nabla h b_h - \nabla^\perp h \tilde{b}_h \cdot \nabla h a_h.
\]

Here, \( \tilde{\cdot} \) represents a mapping from cell centers to cell vertices. Clearly, the discrete Jacobian \( J_h(a_h, b_h) \) is skew-symmetric with respect to its two arguments. This approach is reminiscent of the discrete approximation of the trilinear form \( b(u, v, w) \) arising in the study of the Navier-Stokes equations (see [32]).

With the Jacobian taken care of, the approximation of \( \{ F, H \}_\zeta \zeta \) and \( \{ F, H \}_\gamma \gamma \) is now straightforward,

\[
\{ F, H \}_\zeta \zeta \approx \{ F, H \}_h,\zeta \zeta \equiv \int_M \tilde{q}_h J_h \left( \frac{\delta F}{\delta \zeta_h}, \frac{\delta H}{\delta \zeta_h} \right) dx,
\]

\[
\{ F, H \}_\gamma \gamma \approx \{ F, H \}_h,\gamma \gamma \equiv \int_M \tilde{q}_h J_h \left( \frac{\delta F}{\delta \gamma_h}, \frac{\delta H}{\delta \gamma_h} \right) dx,
\]

where \( \tilde{q}_h \) is the potential vorticity at cell edges, which is a remapping of the PV \( q_h \) at cell centers, and \( q_h \) is defined (see (2.29)) as

\[
q_h = \frac{f + \zeta_h}{\phi_h}.
\]
As pointed out above, the definition of \( \{ F, H \}_{\phi_\zeta \gamma} \) already contains a permutation of its two argument, and this permutation also appears in a straightforward approximation of the expression by the finite difference method,

\[
\{ F, H \}_{\phi_\zeta \gamma} \approx \{ F, H \}_{h, \phi_\zeta \gamma} = 2 \int_\mathcal{M} \hat{q}_h (\nabla_h F_{\gamma h} \cdot \nabla_h H_{\zeta h} - \nabla_h H_{\gamma h} \cdot \nabla_h F_{\zeta h}) \, dx + 2 \int_\mathcal{M} (\nabla_h F_{\gamma h} \cdot \nabla_h H_{\phi h} - \nabla_h H_{\gamma h} \cdot \nabla_h F_{\phi h}) \, dx.
\]

The discrete Poisson bracket is the sum of the three expression given above,

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

We note that this discrete Poisson bracket is skew-symmetric, and independent of the choice of the Hamiltonian \( H \). A discrete scheme based on this Poisson bracket is given by

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

We now derive the evolution equation for the discrete prognostic variables \( \phi_h, \zeta_h, \) and \( \gamma_h \). The approximate Hamiltonian is given in (3.1), and its functional derivatives w.r.t. \( \phi_h, \zeta_h, \) and \( \gamma_h \) have been given in (3.4). These expressions will be used in the discrete Poisson bracket.

First, for an arbitrary cell index \( i \), we take \( F = \zeta_i \). \( F \) can be written as a functional of \( \zeta_h \) with the help of a special kernel function \( \delta_{ih} \) as follows,

\[
F = \int_\mathcal{M} \delta_{ih} \zeta_h \, dx,
\]

where \( \delta_{ih} \) is the discrete Kronecker delta function centered on cell \( i \), i.e.

\[
\delta_{ih} = \sum_j \delta_{ij} \chi_j, \quad \delta_{ij} = \begin{cases} 0 & \text{if } j \neq i, \\ 1 & \text{if } j = i. \end{cases}
\]

Thus, \( F \) as a functional of \( \zeta_h \) has derivatives

\[
\frac{\delta F}{\delta \phi_h} = 0, \quad \frac{\delta F}{\delta \zeta_h} = \delta_{ih}, \quad \frac{\delta F}{\delta \gamma_h} = 0.
\]

Substituting the discrete functional derivatives, given in (3.4) and (3.17), into the sub-bracket \( \{ \zeta_i, H \}_{h, \zeta \zeta} \), one finds that

\[
\{ \zeta_i, H \}_{h, \zeta \zeta} = \int_\mathcal{M} \hat{q}_h \left( -\nabla_h^+ \delta_{ih} \cdot \nabla_h \psi_h + \nabla_h^+ \psi_h \cdot \nabla_h \delta_{ih} \right) \, dx = \frac{1}{2} \int_\mathcal{M} \delta_{ih} \nabla_h \times (\hat{q}_h \nabla_h \psi_h) \, dx - \frac{1}{2} \int_\mathcal{M} \delta_{ih} \nabla_h \cdot \left( \hat{q}_h \nabla_h^+ \psi_h \right) \, dx.
\]

Both integration by parts in the above derivations go through for arbitrary cell index \( i \), thanks to the homogeneous boundary conditions on \( \psi_h \) and \( \bar{\psi}_h \). Applying the adjoint identities (C.2) to the above, we obtain

\[
\{ \zeta_i, H \}_{h, \zeta \zeta} = \frac{1}{2} \left[ \nabla_h \times (\hat{q}_h \nabla_h \psi_h) \right]_i - \frac{1}{2} \left[ \nabla_h \cdot \left( \hat{q}_h \nabla_h^+ \psi_h \right) \right]_i.
\]
Since $F$ is independent of $\gamma_h$, the second component of the Poisson bracket vanishes for this particular quantity, i.e.

\begin{equation}
\{ \zeta_i, H \}_h,\gamma\gamma = 0.
\end{equation}

Finally, substituting the discrete functional derivatives (3.4) and (3.17) into the third component of the Poisson bracket, we have

\begin{equation}
\{ \zeta_i, H \}_h,\phi\zeta\gamma = 2 \int_M \hat{q}_h \nabla_h \delta_{ih} \cdot \nabla_h \chi_h dx
= - \int_M \delta_{ih} \nabla_h \cdot (\hat{q}_h \nabla_h \chi_h) dx.
\end{equation}

The integration-by-parts formula (C.3) has been used. The specification of the discrete Kronecker delta function $\delta_{ih}$ allows us to write this component as

\begin{equation}
\{ \zeta_i, H \}_h,\phi\zeta\gamma = - \left[ \nabla_h \cdot (\hat{q}_h \nabla_h \chi_h) \right]_i.
\end{equation}

For $F = \zeta_i$, the Poisson bracket $\{ F, H \}_h$ is the sum of the expressions (3.18)–(3.20), and the semi-discrete equation for $\zeta_i$ takes the form

\begin{equation}
\frac{d}{dt} \zeta_i = \frac{1}{2} \left[ \nabla_h \times (\hat{q}_h \nabla_h \psi_h) \right]_i
- \frac{1}{2} \left[ \nabla_h \cdot (\hat{q}_h \nabla_h \psi_h) \right]_i
- \left[ \nabla_h \cdot (\hat{q}_h \nabla_h \chi_h) \right]_i.
\end{equation}

The derivation of the evolution equation for the divergence $\gamma_i$ is made more complex by the non-vanishing boundary terms. A guiding principle in handling the boundary terms is that the skew-symmetry of the Poisson brackets should be preserved. We let $F = \gamma_i$, for an arbitrary cell index $i \in \mathcal{C}$. Its functional derivatives are found to be

\begin{equation}
\frac{\delta F}{\delta \phi_h} = 0, \quad \frac{\delta F}{\delta \zeta_h} = 0, \quad \frac{\delta F}{\delta \gamma_h} = \delta_{ih}.
\end{equation}

Since $F$ here is independent of the state variables $\zeta_h$, the first component of the Poisson bracket vanishes, i.e.

\begin{equation}
\{ \gamma_i, H \}_h,\zeta\zeta = 0.
\end{equation}

Substituting the discrete functional derivative $H_{\gamma_h}$ and the discrete functional derivative $F_{\gamma_h} = \delta_{ih}$ into the second components of the Poisson bracket, and obtain

\begin{equation}
\{ \gamma_i, H \}_h,\gamma\gamma = - \int_M \hat{q}_h \nabla_h^\perp \delta_{ih} \cdot \nabla_h \chi_h dx
+ \int_M \hat{q}_h \nabla_h^\perp \chi_h \cdot \nabla_h \delta_{ih} dx.
\end{equation}

If $i \in \mathcal{I}$, i.e. $i$ refers to an interior cell, then $\delta_{ih}$ vanishes on the boundary. We apply the integration-by-parts formula (C.4) to the first inner product above to obtain

\begin{equation}
\int_M \hat{q}_h \nabla_h^\perp \delta_{ih} \cdot \nabla_h \chi_h dx
= - \frac{1}{2} \int_M \delta_{ih} \nabla_h \times (\hat{q}_h \nabla_h \chi_h) dx.
\end{equation}

Applying the adjoint identity (C.2) to the right-hand side, and use the definition for the discrete delta function $\delta_{ih}$, we derive that

\begin{equation}
\int_M \hat{q}_h \nabla_h^\perp \delta_{ih} \cdot \nabla_h \chi_h dx
= - \frac{1}{2} \left[ \nabla_h \times (\hat{q}_h \nabla_h \chi_h) \right]_i.
\end{equation}
We now consider the boundary case when \( i \in \mathcal{BC} \). We let \( i_1 \) and \( i_2 \) be two neighboring boundary cells, with \( i_1, i, i_2 \) ordered in the counter clockwise direction. We designate the two boundary edges of cell \( i \) as \( e_1 \) and \( e_2 \), which are again ordered in the counter clockwise direction (see Figure 3.1). Applying the discrete integration by parts formula (C.4) to the first inner product on the right-hand side of (3.24) and using the fact that \( \widetilde{\delta}_i h \) vanishes everywhere on the boundary except on edges \( e_1 \) and \( e_2 \) around cell \( i \), we have

\[
\int M \hat{q}_h \nabla_h \cdot \nabla_h \chi_h \cdot \nabla_h \delta_i h \cdot \nabla_h \chi_h d\mathbf{x} = -\frac{1}{2} \int M \nabla_h \delta_i h \cdot (\hat{q}_h \nabla_h \chi_h) d\mathbf{x} \\
- \frac{1}{2} \left( \delta_{i,e_1} \hat{q}_{e_1} [\nabla_h \chi_h]_{e_1} d_{e_1} \sum_{\nu \in V E(e_1)} t_{e_1,\nu} + \delta_{i,e_1} \hat{q}_{e_1} [\nabla_h \chi_h]_{e_1} d_{e_1} \sum_{\nu \in V E(e_1)} t_{e_1,\nu} \right).
\]

We approximate the values of \( \tilde{\delta}_i h \) at edge \( e_1 \) and \( e_2 \) by

\[
\delta_{i,e_1} = \delta_{i,e_2} \approx \frac{1}{2} \delta_{i,i} = \frac{1}{2|A_i|}.
\]

Here \(|A_i|\) refers to the area of cell \( i \). We also note that, based on the assumed counterclockwise orientation of \( \{e_1, e_2\} \) and \( \{i_1, i, i_2\} \), we have

\[
\sum_{\nu \in V E(e_1)} t_{e_1,\nu} = n_{e_1,i}, \quad \sum_{\nu \in V E(e_2)} t_{e_2,\nu} = -n_{e_2,i}.
\]

Substituting (3.27) and (3.28), as well as the specification (B.3) for \([\nabla_h \chi_h]_{e_1}\) and \([\nabla_h \chi_h]_{e_2}\) into (3.26), we obtain, for a boundary cell \( i \),

\[
\int M \hat{q}_h \nabla_h \cdot \nabla_h \chi_h d\mathbf{x} = -\frac{1}{2} \left[ \nabla_h \times (\hat{q}_h \nabla_h \chi_h) \right]_{i} \]

\[
+ \frac{1}{4|A_i|} \left( \hat{q}_{e_1} (\chi_i - \chi_{i_1}) + \hat{q}_{e_2} (\chi_{i_2} - \chi_i) \right).
\]

For the second integral on the right-hand side of (3.24), we apply the integration by parts formula (C.3) directly,

\[
\int M \hat{q}_h \nabla_h \cdot \nabla_h \delta_i h d\mathbf{x} = -\frac{1}{2} \int M \nabla_h \cdot (\hat{q}_h \nabla_h \chi_h) \delta_i h d\mathbf{x} = -\frac{1}{2} \left[ \nabla_h \cdot (\hat{q}_h \nabla_h \chi_h) \right]_{i}.
\]
Combining (3.24)-(3.30), we conclude that

\[ \{ \gamma_i, H \}_{h, \gamma} = \begin{cases} \frac{1}{2} \left[ \nabla_h \times (\tilde{q}_h \nabla_h \chi_h) \right]_i - \frac{1}{2} \left[ \nabla_h \cdot (\tilde{q}_h \nabla_h \chi_h) \right]_i, & \text{if } i \in IC, \\ \text{(same from above)} - \frac{1}{4|A_i|} \left( \tilde{q}_e_1 (\chi_i - \chi_i) + \tilde{q}_e_2 (\chi_i - \chi_i) \right), & \text{if } i \in BC. \end{cases} \]

Substituting the discrete functional derivatives (3.4) of \( H \) and the discrete functional derivatives (3.22) of \( \gamma_i \) into the third component of the Poisson bracket (3.13), one obtains

\[ \{ \gamma_i, H \}_{h, \phi_{\zeta \gamma}} = -2 \int_M \tilde{q}_h \nabla_h \delta_{ih} \cdot \nabla_h \psi_h dx + 2 \int_M \nabla_h \delta_{ih} \cdot \nabla_h \Phi_h dx. \]

Applying the integration by parts formula (C.3) to both inner products in the above, one reaches at

\[ \{ \gamma_i, H \}_{h, \phi_{\zeta \gamma}} = \left[ \nabla_h \cdot (\tilde{q}_h \nabla_h \psi_h) \right]_i - \Delta_h \Phi_h. \]

The Poisson bracket for \( F = \gamma_i \) is a sum of all three expressions in (3.23), (3.31), and (3.33). For interior cells \((i \in IC)\), the semi-discrete evolution equation for this quantity has the form

\[ \frac{d}{dt} \gamma_i = \left[ \nabla_h \cdot (\tilde{q}_h \nabla_h \psi_h) \right]_i + \frac{1}{2} \left[ \nabla_h \times (\tilde{q}_h \nabla_h \chi_h) \right]_i - \frac{1}{2} \left[ \nabla_h \cdot (\tilde{q}_h \nabla_h \chi_h) \right]_i - |\Delta_h \Phi_h|_i. \]

For boundary cells \((i \in BC)\),

\[ \frac{d}{dt} \gamma_i = \left[ \nabla_h \cdot (\tilde{q}_h \nabla_h \psi_h) \right]_i + \frac{1}{2} \left[ \nabla_h \times (\tilde{q}_h \nabla_h \chi_h) \right]_i - \frac{1}{2} \left[ \nabla_h \cdot (\tilde{q}_h \nabla_h \chi_h) \right]_i - |\Delta_h \Phi_h|_i - \frac{1}{4|A_i|} \left( \tilde{q}_e_1 (\chi_i - \chi_i) + \tilde{q}_e_2 (\chi_i - \chi_i) \right). \]

Finally, by taking \( F = \phi_i \), we have

\[ \frac{\delta F}{\delta \phi_h} = \delta_{ih}, \quad \frac{\delta F}{\delta \chi_h} = 0, \quad \frac{\delta F}{\delta \gamma_h} = 0. \]

The three components of the Poisson bracket for this quantity can be calculated as before,

\[ \{ \phi_i, H \}_{h, \zeta \zeta} = 0, \]
\[ \{ \phi_i, H \}_{h, \gamma \gamma} = 0, \]
\[ \{ \phi_i, H \}_{h, \phi \gamma} = -\Delta_h \chi_h. \]

The Poisson bracket for \( F = \phi_i \) is the sum of these expressions, and the semi-discrete evolution equation for it can be simply written as

\[ \frac{d}{dt} \phi_i = -[\Delta_h \chi_h]_i. \]
For reference, we summarize the full energy-conserving semi-discrete scheme for the shallow water equations as follows,

\[
\begin{align*}
\frac{d}{dt} \phi_i &= - [\Delta_h \chi h], \\
\frac{d}{dt} \zeta_i &= \frac{1}{2} \left[ \nabla_h \times (\bar{q}_h \nabla_h \psi_h) \right]_i - \frac{1}{2} \left[ \nabla_h \cdot \left( \bar{q}_h \nabla_h \psi_h \right) \right]_i - \left[ \nabla_h \cdot \left( \bar{q}_h \nabla_h \chi_h \right) \right]_i, \\
\frac{d}{dt} \gamma_i &= \frac{1}{2} \left[ \nabla_h \times (\bar{q}_h \nabla_h \chi_h) \right]_i - \frac{1}{2} \left[ \nabla_h \cdot \left( \bar{q}_h \nabla_h x \chi_h \right) \right]_i + \left[ \nabla_h \cdot \left( \bar{q}_h \nabla_h \psi_h \right) \right]_i - [\Delta_h \Phi_h]_i - \frac{1}{4 |A_i|} (\tilde{q}_{e1} (\chi_i - \chi_{i1}) + \tilde{q}_{e2} (\chi_{i2} - \chi_i)).
\end{align*}
\]

(3.41)

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

A discrete analogue of Theorem 2.1 can also be established.

**Theorem 3.1.** An arbitrary functional \(F = F(\phi_h, \zeta_h, \gamma_h)\) of the discrete state variables evolves according to the equation (3.14).

The proof of this theorem relies on the specific form of the discrete Poisson bracket (3.13), and unlike for the analytical case, the boundary terms will show up during the process of integration by parts.

**Proof of Theorem 3.1.** We let \(F = F(\phi_h, \zeta_h, \gamma_h)\) be an arbitrary functional of the state variables, which does not explicitly depend on time \(t\). We proceed as in the analytical case, and find the variation of this functional,

\[
\delta F = \int_{\mathcal{M}} \left( \frac{\delta F}{\delta \phi_h} \delta \phi_h + \frac{\delta F}{\delta \zeta_h} \delta \zeta_h + \frac{\delta F}{\delta \gamma_h} \delta \gamma_h \right) d\mathbf{x}.
\]

Dividing both sides by \(\delta t\), and noticing that the state variables \(\phi_h, \zeta_h, \) and \(\gamma_h\) each satisfies the evolution equation (3.14), one obtains

\[
\frac{dF}{dt} = \int_{\mathcal{M}} \left( \frac{\delta F}{\delta \phi_h} (\phi_h, H)_h + \frac{\delta F}{\delta \zeta_h} (\zeta_h, H)_h + \frac{\delta F}{\delta \gamma_h} (\gamma_h, H)_h \right) d\mathbf{x}.
\]

(3.42)

We now separately examine the terms involved in the above. We first observe that \(\phi_h\) is independent of the other two state variables, and therefore

\[
\int_{\mathcal{M}} \frac{\delta F}{\delta \phi_h} (\phi_h, H)_h d\mathbf{x} = \int_{\mathcal{M}} \frac{\delta F}{\delta \phi_h} (\phi_h, H)_{\phi \gamma} d\mathbf{x} = \sum_{i \in \mathcal{C}} \left[ \frac{\delta F}{\delta \phi_h} \right]_i \int_{\mathcal{M}} (-2) \nabla_h \delta_{ih} \cdot \nabla_h \left( \frac{\delta H}{\delta \gamma_h} \right) d\mathbf{y} |A_i|.
\]

Integration by parts in \(\mathbf{y}\), and then switching the summation with the integration, one has

\[
\int_{\mathcal{M}} \frac{\delta F}{\delta \phi_h} (\phi_h, H)_h d\mathbf{x} = \int_{\mathcal{M}} \nabla_h \cdot \left( \nabla_h \left( \frac{\delta H}{\delta \gamma_h} \right) \right) \left( \sum_{i \in \mathcal{C}} \left[ \frac{\delta F}{\delta \phi_h} \right]_i \delta_{ih}(\mathbf{y}) |A_i| \right) d\mathbf{y}.
\]

The Kronecker-delta function \(\delta_{ih}\) with respect to index \(i\) is defined in (3.16). The summation over \(i\) yields a discrete scalar field \(\delta F/\delta \phi_h\) with the dependent variable \(\mathbf{y}\).
Thus, one has

$$\int_M \frac{\delta F}{\delta \phi_h} \{\phi_h, H\}_h dx = \int_M \nabla_h \left( \frac{\delta H}{\delta \gamma_h} \right) \cdot \frac{\delta F}{\delta \phi_h} (y) dy.$$ 

Integrating by parts again in $y$, one finds that

$$\int_M \frac{\delta F}{\delta \phi_h} \{\phi_h, H\}_h dx = \int_M -2 \nabla_h \left( \frac{\delta F}{\delta \phi_h} (y) \right) \cdot \nabla_h \left( \frac{\delta H}{\delta \gamma_h} \right) dy.$$ 

Turning our attention to the second term on the right-hand side of (3.42), we note that $\zeta_h$ is independent of $\gamma_h$ and $\phi_h$, and therefore,

$$\int_M \frac{\delta F}{\delta \phi_h} \{\zeta_h, H\}_h dx = \int_M \frac{\delta F}{\delta \zeta_h} \{\zeta_h, H\}_h, \zeta \zeta d \gamma_h + \{\zeta_h, H\}_h, \phi \gamma d \gamma_h.$$ 

The treatment of each of the two terms on the right-hand side above follows the same procedure just presented, involving integration by parts and switching the integrations and summations. One has, for the first term above,

$$\int_M \frac{\delta F}{\delta \phi_h} \{\zeta_h, H\}_h, \gamma \gamma d \gamma_h =$$

$$\int_M \left( \hat{q}_h \nabla_h \left( \frac{\delta F}{\delta \phi_h} \right) \cdot \nabla_h \left( \frac{\delta H}{\delta \zeta_h} \right) - \hat{q}_h \nabla_h \left( \frac{\delta F}{\delta \zeta_h} \right) \cdot \nabla_h \left( \frac{\delta H}{\delta \gamma_h} \right) \right) dx \equiv \{F, H\}_h, \gamma \gamma.$$ 

For the second term, one has

$$\int_M \frac{\delta F}{\delta \phi_h} \{\zeta_h, H\}_h, \phi \gamma d \gamma_h = \int_M (-2) \hat{q}_h \nabla_h \left( \frac{\delta F}{\delta \zeta_h} \right) \cdot \nabla_h \left( \frac{\delta H}{\delta \gamma_h} \right) dx.$$ 

Substituting (3.45) and (3.46) into (3.44), one therefore has

$$\int_M \frac{\delta F}{\delta \phi_h} \{\zeta_h, H\}_h dx = \{F, H\}_h, \gamma \gamma + \int_M (-2) \hat{q}_h \nabla_h \left( \frac{\delta F}{\delta \zeta_h} \right) \cdot \nabla_h \left( \frac{\delta H}{\delta \gamma_h} \right) dx.$$ 

The variable $\gamma_h$ is independent of $\zeta_h$ and $\phi_h$, and therefore the third term on the right-hand side of (3.42) is split into two terms,

$$\int_M \frac{\delta F}{\delta \phi_h} \{\gamma_h, H\}_h dx = \int_M \frac{\delta F}{\delta \gamma_h} \{\gamma_h, H\}_h, \gamma \gamma + \{\gamma_h, H\}_h, \phi \gamma d \gamma_h.$$ 

Calculation of the first term on the right-hand side is the most complex, as it involves non-zero boundary terms. We expand this term using the specification for the Poisson bracket component $\{\cdot, \cdot\}_h, \gamma \gamma$ and by replacing integration in $y$ with a discrete summation,

$$\int_M \frac{\delta F}{\delta \gamma_h} \{\gamma_h, H\}_h, \gamma \gamma =$$

$$\sum_{i \in C} |A_i| \left( \int_M \hat{q}_h \nabla_h \tilde{\gamma}_h \cdot \nabla_h (-\gamma_h) dy - \int_M \hat{q}_h \nabla_h \tilde{\gamma}_h \cdot \nabla_h \delta_{ih} dy \right).$$
As demonstrated in (3.25) or (3.29), integration by parts on the first integral has different outcomes, depending on whether $i \in IC$ (interior cells) or $i \in BC$ (boundary cells). More specifically,

$$\int_{\mathcal{M}} \hat{q}_h \nabla_h^\perp \delta h \cdot \nabla_h (-\chi_h) dy = \frac{1}{2} \int_{\mathcal{M}} \delta h \nabla_h \times (\hat{q}_h \nabla_h \chi_h) dy$$

$$+ \begin{cases} 
0 & \text{if } i \in IC, \\
-\frac{1}{4|A_i|} (\hat{q}_{e_1} (\chi_i - \chi_{i_1}) + \hat{q}_{e_2} (\chi_{i_2} - \chi_{i})) & \text{if } i \in BC.
\end{cases}$$

For the boundary case, the geometric relations between $i, i_1, i_2, e_1$ and $e_2$ are as depicted in Figure 3.1.

Therefore, the summation involving the first integral on the right-hand side of (3.49) can be written as

$$\sum_{i \in C} |A_i| \left[ \frac{\delta F}{\delta \phi_h} \right]_i \int_{\mathcal{M}} \hat{q}_h \nabla_h^\perp \delta h \cdot \nabla_h (-\chi_h) dy = \sum_{i \in C} |A_i| \left[ \frac{\delta F}{\delta \phi_h} \right]_i \int_{\mathcal{M}} \frac{1}{2} \delta h \nabla_h \times (\hat{q}_h \nabla_h \chi_h) dy - \sum_{i \in BC} \left[ \frac{\delta F}{\delta \gamma_h} \right]_i \frac{\hat{q}_{e_1} (\chi_i - \chi_{i_1}) + \hat{q}_{e_2} (\chi_{i_2} - \chi_i)}{4|A_i|} \cdot |A_i|.$$  

One switches the summation and the integration on the first term on the right-hand side, and then applies the adjoint identity to obtain

$$\sum_{i \in C} |A_i| \left[ \frac{\delta F}{\delta \phi_h} \right]_i \int_{\mathcal{M}} \hat{q}_h \nabla_h^\perp \delta h \cdot \nabla_h (-\chi_h) dy = \int_{\mathcal{M}} \frac{1}{2} \left[ \frac{\delta F}{\delta \phi_h} \right] \nabla_h \times (\hat{q}_h \nabla_h \chi_h) dy - \frac{1}{4} \sum_{i \in BC} \left[ \frac{\delta F}{\delta \gamma_h} \right]_i (\hat{q}_{e_1} (\chi_i - \chi_{i_1}) + \hat{q}_{e_2} (\chi_{i_2} - \chi_i)).$$

For the first term on the right-hand side, one applies the discrete integration (C.4), and obtains

$$\int_{\mathcal{M}} \frac{1}{2} \left[ \frac{\delta F}{\delta \phi_h} \right] \nabla_h \times (\hat{q}_h \nabla_h \chi_h) dy = - \int_{\mathcal{M}} \hat{q}_h \nabla_h^\perp \left( \frac{\delta F}{\delta \gamma_h} \right) \cdot \nabla_h \chi_h dy$$

$$- \frac{1}{2} \sum_{e \in \mathcal{E}B} \left[ \frac{\delta F}{\delta \gamma_h} \right]_e \hat{q}_e [\nabla_h \chi_h]_e d_e \sum_{e \in \mathcal{V}(e)} t_{e,v}.$$
substituting these definitions into the summation above on the boundary, one obtains

\[
\int_M \frac{1}{2} \frac{\delta F}{\delta \phi_h} \nabla_h \times (\tilde{q}_h \nabla_h \chi_h) dy = - \int_M \tilde{q}_h \nabla_h^\bot \left( \frac{\delta F}{\delta \gamma_h} \right) \cdot \nabla_h \chi_h dy + \sum_{e \in \partial E} \left( \sum_{i \in \partial E(i)} \tilde{q}_e \sum_{\nu \in \partial E} \chi_i n_{e,i} \sum_{\nu \in \partial E} t_{e,\nu} \right).
\]

Switching the two outermost summations, one have

\[
\int_M \frac{1}{2} \frac{\delta F}{\delta \phi_h} \nabla_h \times (\tilde{q}_h \nabla_h \chi_h) dy = - \int_M \tilde{q}_h \nabla_h^\bot \left( \tilde{\delta} \chi_h \right) \cdot \nabla_h \chi_h dy + \frac{1}{4} \sum_{i \in \partial C} \left( \sum_{e \in \partial E \cap \partial C(i)} \tilde{q}_e \sum_{\nu \in \partial E} \chi_i n_{e,i} \sum_{\nu \in \partial E} t_{e,\nu} \right).
\]

One notes that the term in the parentheses represent a difference formula in the positive orientation, i.e. counter-clockwise direction, on the boundary. Thus, with boundary cells \((i_1, i, i_2)\) ordered in the counter-clockwise direction, one can write the terms as

\[
\int_M \frac{1}{2} \frac{\delta F}{\delta \phi_h} \nabla_h \times (\tilde{q}_h \nabla_h \chi_h) dy = - \int_M \tilde{q}_h \nabla_h^\bot \left( \tilde{\delta} \chi_h \right) \cdot \nabla_h \chi_h dy + \frac{1}{4} \sum_{i \in \partial C} \left( \tilde{q}_{e_1} (\chi_i - \chi_{i_1}) + \tilde{q}_{e_2} (\chi_{i_2} - \chi_i) \right).
\]

One notices that the boundary terms exactly match the boundary terms in (3.51). Therefore, substituting the expression on the right-hand side into (3.51), one greatly simplifies it into

\[
\sum_{i \in \partial C} |A_i| \left( \int_M \tilde{q}_h \nabla_h^\bot \tilde{\delta} \chi_h \cdot \nabla_h (-\chi_h) dy = - \int_M \tilde{q}_h \nabla_h^\bot \left( \tilde{\delta} \chi_h \right) \cdot \nabla_h \chi_h dy. \right.
\]

The summation on the right-hand side of (3.49) can be handled in the usual way, with no complications from the boundary terms, and one has

\[
\sum_{i \in \partial C} |A_i| \left( \int_M \tilde{q}_h \nabla_h^\bot \tilde{\delta} \chi_h \cdot \nabla_h \tilde{\delta} \chi_h dy = - \int_M \tilde{q}_h \nabla_h^\bot \left( \tilde{\delta} \chi_h \right) \cdot \nabla_h \tilde{\delta} \chi_h dy. \right.
\]

With (3.52) and (3.53), one therefore concludes from (3.49) that

\[
\int_M \frac{\delta F}{\delta \gamma_h} (\gamma_h, H)_{\gamma,\gamma} = \{ F, H \}_{\gamma,\gamma}.
\]

The treatment of the second term on the right-hand side of (3.48) is straightforward without complications from the boundary terms. One starts by replacing
\{\gamma_h, H\}^{h, \phi \zeta \gamma}_h \text{ by its definition (3.12), and noticing that } \gamma_h \text{ is independent of } \phi_h \text{ and } \zeta_h, \text{ one has }

\[ \int_{\mathcal{M}} \frac{\delta F}{\delta \gamma_h} \{\gamma_h, H\}^{h, \phi \zeta \gamma}_h \, dx = \sum_{i \in C} |A_i| \left[ \int_{\mathcal{M}} \left( 2 \tilde{q}_h \nabla_h \delta_{ih} \cdot \nabla_h \frac{\delta H}{\delta \gamma_h} + 2 \nabla \delta_{ih} \nabla_h \cdot \Phi_h \right) \right] dy. \]

For both integrals, the discrete integration by parts formula (C.3) applies without generating any boundary terms. Afterwards, one proceeds by switching the summation and the integration, and applying the discrete integration by parts formula again, then one has in the end

(3.55)

\[ \int_{\mathcal{M}} \frac{\delta F}{\delta \gamma_h} \{\gamma_h, H\}^{h, \phi \zeta \gamma}_h \, dx = \int_{\mathcal{M}} \left( 2 \tilde{q}_h \nabla_h \frac{\delta F}{\delta \gamma_h} \cdot \nabla_h \frac{\delta H}{\delta \zeta_h} + 2 \nabla \frac{\delta F}{\delta \gamma_h} \cdot \nabla_h \Phi_h \right) \, dy. \]

From (3.48), (3.54), and (3.55), one concludes that

(3.56)

\[ \int_{\mathcal{M}} \frac{\delta F}{\delta \gamma_h} \{\gamma_h, H\}^{h, \phi \zeta \gamma}_h \, dx = \{F, H\}^{h, \gamma \gamma}_h + \int_{\mathcal{M}} \left( 2 \tilde{q}_h \nabla_h \frac{\delta F}{\delta \gamma_h} \cdot \nabla_h \frac{\delta H}{\delta \zeta_h} + 2 \nabla \frac{\delta F}{\delta \gamma_h} \cdot \nabla_h \Phi_h \right) \, dy. \]

Taking (3.43), (3.47), and (3.56) into the evolutionary equation (3.42), one has

\[ \frac{dF}{dt} = \{F, H\}^{h, \zeta \zeta}_h + \{F, H\}^{h, \gamma \gamma}_h + \int_{\mathcal{M}} \left( 2 \tilde{q}_h \nabla_h \frac{\delta F}{\delta \gamma_h} \cdot \nabla_h \frac{\delta H}{\delta \zeta_h} + 2 \nabla \frac{\delta F}{\delta \gamma_h} \cdot \nabla_h \Phi_h \right) \, dy. \]

One notes that the integral terms above constitutes the definition of the component \{\cdot, \cdot\}^{h, \phi \zeta \gamma}_h of the Poisson bracket, which together with the other two components already present in the equation, constitutes the definition of the Poisson bracket itself, and therefore one finally has

(3.57)

\[ \frac{dF}{dt} = \{F, H\}^{h}_h. \]

This equation holds for an arbitrary functional of the discrete variables \phi_h, \zeta_h, \text{ and } \gamma_h. \quad \Box

The result that the scheme (3.41) conserves the total energy, which is a functional of the discrete state variables, is then a simple consequence of the skew-symmetry of the discrete Poisson bracket \{\cdot, \cdot\}^h.

We now examine the conservation of quantities in the form of

(3.58)

\[ C = \int_{\mathcal{M}} \phi_h G(q_h) \, dx. \]
When $G(q_h) = q_h$, $C = \int_{\mathcal{M}} \phi_h q_h d\mathbf{x}$ is the mass. Concerning its functional derivatives, one finds
\[ \frac{\delta C}{\delta \phi_h} = 1, \quad \frac{\delta C}{\delta \zeta_h} = 0, \quad \frac{\delta C}{\delta \gamma_h} = 0. \]
Substituting $C$ as $F$ into the Poisson bracket (3.13), one has
\[ \{C, H\}_h = \int_{\mathcal{M}} -2 \nabla_h C \phi_h \cdot \nabla_h H \gamma_h d\mathbf{x} = 0. \]
Hence, the mass is conserved in the scheme (3.41).

When $G(q_h) = q_h$, $C = \int_{\mathcal{M}} \phi_h q_h d\mathbf{x} = \int_{\mathcal{M}} (f + \zeta_h) d\mathbf{x}$ is the circulation. It has functional derivatives
\[ \frac{\delta C}{\delta \phi_h} = 0, \quad \frac{\delta C}{\delta \zeta_h} = 1, \quad \frac{\delta C}{\delta \gamma_h} = 0. \]
Substituting these functional derivatives into the Poisson bracket (3.13), one has
\[ \{F, H\}_h = \int_{\mathcal{M}} \hat{q}_h \left( \nabla_h \tilde{C}_{\zeta_h} \cdot \nabla_h H \zeta_h - \nabla_h \tilde{H}_{\zeta_h} \cdot \nabla_h \tilde{C}_{\zeta_h} - 2 \nabla_h C \zeta_h \cdot \nabla_h H \gamma_h \right) d\mathbf{x} = 0. \]
Hence the total circulation is also conserved.

When $G(q_h) = q_h^2/2$, $C = \int_{\mathcal{M}} \phi_h q_h^2/2 d\mathbf{x}$ is the discrete potential enstrophy. We note that the PV $q_h$ is given by $q_h = (f + \zeta_h)/\phi_h$. Thus, the discrete potential enstrophy also takes the form $C = \int_{\mathcal{M}} \hat{\phi}_h^{-1} (f + \zeta_h)^2 d\mathbf{x}$. It has functional derivatives
\[ \frac{\delta C}{\delta \phi_h} = -\frac{1}{2} q_h^2, \quad \frac{\delta C}{\delta \zeta_h} = q_h, \quad \frac{\delta C}{\delta \gamma_h} = 0. \]
Due to the independence of the quantity $C$ from the divergence $\gamma_h$, its Poisson bracket has only two components that might be non-zero,
\[ \{C, H\}_h = \{C, H\}_{h,\zeta} + \{C, H\}_{h,\phi \gamma}, \]
Substituting the functional derivatives of $C$ and $H$ into the first component, one has
\[ \{C, H\}_{h,\zeta} = \int_{\mathcal{M}} \tilde{q}_h \left( \nabla_h \tilde{C}_{\zeta_h} \cdot \nabla_h H \zeta_h - \nabla_h \tilde{H}_{\zeta_h} \cdot \nabla_h \tilde{C}_{\zeta_h} \right) d\mathbf{x}. \]
With the mapping $\tilde{\cdot}$ defined as in (B.2a), the second term in the integral above vanishes, for
\[ \int_{\mathcal{M}} \tilde{q}_h \nabla_h \tilde{H}_{\zeta_h} \cdot \nabla_h q_h d\mathbf{x} = \int_{\mathcal{M}} \nabla_h \tilde{H}_{\zeta_h} \cdot \nabla_h \left( \frac{1}{2} q_h^2 \right) d\mathbf{x} = 0, \]
by the virtue of Lemma C.4. Thus, one has
\[ \{C, H\}_{h,\zeta} = \int_{\mathcal{M}} \tilde{q}_h \nabla_h \tilde{q}_h \cdot \nabla_h H \zeta_h. \]
One notes that one can modify the specification (B.2a) of the mapping $\tilde{\cdot}$ to make this remaining term vanishes. But then the other term will not. There is no known
method to make both terms go away, which is just one sign of the limitations of a
discrete system with a finite number of degrees of freedom.

Concerning the second term on the right-hand side of (3.59), one has, after sub-
stituting in the functional derivatives of \( C \),
\[
\{ C, H \}_{h,\phi\gamma} = -2 \int_M \left( \hat{q}_h \nabla_h \hat{q}_h \cdot \nabla_h H_{\gamma_h} + \nabla_h \left( -\frac{1}{2} q_h^2 \right) \cdot \nabla_h H_{\gamma_h} \right) dx.
\]
Again, thanks to the specification (B.2a) of the mapping \( \hat{\cdot} \), one can bring \( \hat{q}_h \) inside
the gradient operator, and arrives at
\[
\{ C, H \}_{h,\phi\gamma} = -2 \int_M \left( \nabla_h \left( \frac{1}{2} q_h^2 \right) \cdot \nabla_h H_{\gamma_h} - \nabla_h \left( \frac{1}{2} q_h^2 \right) \cdot \nabla_h H_{\gamma_h} \right) dx = 0.
\]
Combining (3.60) and (3.61) with (3.59), one concludes that
\[
\{ C, H \}_h = \int_M \hat{q}_h \nabla_h \hat{q}_h \cdot \nabla_h H_{\gamma_h},
\]
which means that the potential enstrophy is not conserved under the scheme (3.41).

### 3.3. An energy and enstrophy conserving scheme.

As just pointed out, the scheme (3.41) fails to conserve the enstrophy. The Nambu bracket ([17]) expands
the Poisson bracket to include the potential enstrophy as a third argument. Then,
the conservation of potential enstrophy is simply a consequence of the skew-symmetry
of the expanded bracket. However, as already pointed out by Salmon ([28]), it is, in
general, difficult to incorporate boundary conditions into the Nambu bracket.

We note that the only reason that the scheme (3.41) fails to conserve the potential
enstrophy is that the first component \( \{ \cdot, \cdot \}_{h,\phi\gamma} \) of the discrete Poisson bracket does
not vanish when the functional \( F \) is taken as the discrete potential enstrophy, unlike
in the analytical case. Thus, we propose to replace this component by a Nambu-style
trinilinear bracket, containing the potential enstrophy as a third functional argument,
which vanishes when the functional \( F \) is taken as the potential enstrophy. The is-
ssue concerning boundary conditions is not a problem here due to the fact that the
streamfunction \( \psi \) vanishes along the boundary (homogeneous Dirichlet).

We shall first consider the analytical case, and then we deal with its discretization.
We let
\[
Z = \int_M \frac{1}{2} \phi q^2 dx.
\]
As we have seen, this quantity has functional derivatives
\[
\frac{\delta Z}{\delta \phi_h} = -\frac{1}{2} q_h^2, \quad \frac{\delta Z}{\delta q_h} = q, \quad \frac{\delta Z}{\delta \gamma_h} = 0.
\]
Using this new variable, the component \( \{ F, H \}_{\phi\gamma} \) of the Poisson bracket can be written as
\[
\{ F, H \}_{\phi\gamma} = \int_M Z_{\phi} \nabla \cdot \nabla H_{\gamma} dx.
\]
We define the right-hand side as a trilinear bracket,

\[(3.64) \{F, H, Z\}_{\zeta\zeta\zeta} = \int_M Z \nabla^\perp F \cdot \nabla H \, d\mathbf{x}.\]

Through a simple exercise and thanks to the homogeneous Dirichlet boundary conditions on the streamfunction \(\psi = -H_\zeta\), one can show that the trilinear bracket (3.64) is skew-symmetric with respect to any two of the arguments, i.e.,

\[(3.65) \{F, H, Z\}_{\zeta\zeta\zeta} = -\{Z, H, F\}_{\zeta\zeta\zeta} = -\{F, Z, H\}_{\zeta\zeta\zeta}.\]

That the Poisson bracket component \(\{F, H\}_{\zeta\zeta}\) vanishes, when \(F\) takes the value of the potential enstrophy \(Z\), is a direct consequence of the skew-symmetry of the trilinear bracket. Also due to the skew-symmetry, the trilinear bracket is invariant under even permutations, i.e.,

\[(3.66) \{F, H, Z\}_{\zeta\zeta\zeta} = \{Z, F, H\}_{\zeta\zeta\zeta} = \{H, Z, F\}_{\zeta\zeta\zeta}.\]

One notes that it is also possible to expand the other two components of the Poisson bracket into trilinear brackets, but it becomes problematic to establish the skew-symmetry and the invariance under even permutations for them, due to the complications from the boundary values. Hence in this work we refrain from adopting the full Nambu bracket for the shallow water equations.

We now turn to the discretization of the trilinear bracket (3.64). The goal here is to preserve the skew-symmetry of the trilinear bracket. This is much harder than the case of the bilinear bracket, because there are more arguments present at the same time. However, with the skew-symmetry property of the trilinear bracket (3.64) and its invariance under even permutation, one can easily derive the relation

\[(3.67) \{F, H, Z\}_{\zeta\zeta\zeta} = \frac{1}{6} (\{F, H, Z\}_{\zeta\zeta\zeta} + \{Z, H, F\}_{\zeta\zeta\zeta} + \{H, Z, F\}_{\zeta\zeta\zeta} - \{H, F, Z\}_{\zeta\zeta\zeta} - \{Z, H, F\}_{\zeta\zeta\zeta} - \{F, Z, H\}_{\zeta\zeta\zeta}).\]

Notes that the right-hand side of (3.67) contains all the possible permutations of \(\{F, H, Z\}_{\zeta\zeta\zeta}\), with the even ones taking the positive signs and the odd ones taking the negative signs. This relation is trivial analytically, but numerically, the expression on the right-hand has a crucial advantage compared with the one on the left-hand side, namely, no matter how each individual term on the right-hand side is discretized, the whole expression will remain skew-symmetric, as long as the permutations are preserved. This observation was already made by Salmon in [26]. Hence, we will construct a discretization of the expression on the right-hand side of (3.67), as an approximation to the trilinear bracket (3.64) and the Poisson bracket component (2.28a).

The discrete Hamiltonian will remain the same as before, as in (3.1). The potential enstrophy (3.63) is approximated by its discrete analogue

\[(3.68) Z = \int_M \frac{1}{2} \phi_h q_h^2 \, d\mathbf{x}.\]

As shown already in the previous section, this quantity has functional derivatives

\[\frac{\delta Z}{\delta \phi_h} = \frac{1}{2} q_h^2, \quad \frac{\delta Z}{\delta \zeta_h} = q_h, \quad \frac{\delta Z}{\delta \gamma_h} = 0.\]
The trilinear bracket \( \{ F, H, Z \}_{\zeta \xi \xi} \), as a single component on the right-hand side of (3.67), is approximated by

\[
\{ F, H, Z \}_{\zeta \xi \xi} = 2 \int_M \hat{Z}_{\zeta \xi} \nabla^\perp_h \hat{F}_{\zeta \xi} \cdot \nabla_h H_{\zeta \xi} \, dx.
\]

Thus, an discretization of the trilinear bracket \( \{ F, H, Z \}_{\zeta \xi \xi} \) itself, as well as the Poisson bracket component \( \{ F, H \}_{\zeta \xi} \), can be constructed by permuting the variables, using (3.67),

\[
\{ F, H \}_{\zeta \xi} = \{ F, H, Z \}_{\zeta \xi \xi} = \frac{1}{3} \left( \int_M \hat{Z}_{\zeta \xi} \nabla^\perp_h \hat{F}_{\zeta \xi} \cdot \nabla_h H_{\zeta \xi} \, dx + \int_M \hat{H}_{\zeta \xi} \nabla^\perp_h \hat{Z}_{\zeta \xi} \cdot \nabla_h F_{\zeta \xi} \, dx + \int_M \hat{F}_{\zeta \xi} \nabla^\perp_h \hat{H}_{\zeta \xi} \cdot \nabla_h Z_{\zeta \xi} \, dx - \int_M \hat{Z}_{\zeta \xi} \nabla^\perp_h \hat{H}_{\zeta \xi} \cdot \nabla_h F_{\zeta \xi} \, dx - \int_M \hat{F}_{\zeta \xi} \nabla^\perp_h \hat{Z}_{\zeta \xi} \cdot \nabla_h H_{\zeta \xi} \, dx - \int_M \hat{H}_{\zeta \xi} \nabla^\perp_h \hat{F}_{\zeta \xi} \cdot \nabla_h Z_{\zeta \xi} \, dx + \int_M \hat{H}_{\zeta \xi} \nabla^\perp_h \hat{Z}_{\zeta \xi} \cdot \nabla_h F_{\zeta \xi} \, dx + \int_M \hat{F}_{\zeta \xi} \nabla^\perp_h \hat{H}_{\zeta \xi} \cdot \nabla_h Z_{\zeta \xi} \, dx + \int_M \hat{Z}_{\zeta \xi} \nabla^\perp_h \hat{H}_{\zeta \xi} \cdot \nabla_h F_{\zeta \xi} \, dx \right).
\]

The key to ensure the skew-symmetry of the discrete trilinear bracket \( \{ \cdot, \cdot, \cdot \}_{\zeta \xi \xi} \) is the consistency in the operation \( \nabla_h (\cdot) \) when applied to different quantities. This operation is defined in (B.6).

This trilinear bracket \( \{ \cdot, \cdot, \cdot \}_{\zeta \xi \xi} \) replaces the bilinear bracket \( \{ \cdot, \cdot \}_{\zeta \xi} \) in the discrete Poisson bracket, i.e.

\[
\{ F, H \}_h = \{ F, H, Z \}_{\zeta \xi \xi} + \{ F, H \}_{\gamma \gamma} + \{ F, H \}_{\phi \gamma}.
\]

The second and third components are as defined in (3.10) and (3.12), respectively. The numerical scheme is again obtained from the single scalar evolution equation

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

We note that the change from the bilinear bracket \( \{ \cdot, \cdot \}_{\zeta \xi} \) to the trilinear bracket \( \{ \cdot, \cdot, \cdot \}_{\zeta \xi \xi} \) only affects part of the equation for \( \zeta_h \), and the equations for \( \gamma_h \) and \( \phi_h \) remain unchanged. We now derive the new equation for \( \zeta_h \). Let us set

\[ F = \zeta_i. \]

Then, as shown before, we have

\[
\frac{\delta F}{\delta \zeta_h} = \delta_{ih}.
\]

Substituting this expression, together with the functional derivatives of \( H \) and \( Z \), into (3.69), one obtains

\[
\{ \zeta_i, H \}_{\zeta \xi} = \{ \zeta_i, H, Z \}_{\zeta \xi \xi} = \frac{1}{3} \left( - \int_M \hat{q}_h \nabla^\perp_h \hat{\psi}_h \cdot \nabla_h q_h \, dx - \int_M \hat{\psi}_h \nabla^\perp_h \hat{q}_h \cdot \nabla_h \delta_{ih} \, dx - \int_M \delta_{ih} \nabla^\perp_h \hat{\psi}_h \cdot \nabla_h q_h \, dx + \int_M \hat{q}_h \nabla^\perp_h \hat{\psi}_h \cdot \nabla_h \delta_{ih} \, dx + \int_M \hat{\psi}_h \nabla^\perp_h \delta_{ih} \cdot \nabla_h q_h \, dx + \int_M \delta_{ih} \nabla^\perp_h \hat{q}_h \cdot \nabla_h \psi_h \, dx \right).
\]
Applying the discrete integration by parts formulas (C.3) and (C.4), and thanks to the adjoint identities (C.1) and (C.2), and to the homogeneous Dirichlet boundary conditions on the discrete streamfunction \( \psi_h \), one reaches at

\[
(3.73) \quad \{ \zeta_i, H, Z \}_h = \frac{1}{6} \left[ \nabla_h \times \left( \tilde{q}_h \nabla_h \psi_h - \tilde{\psi}_h \nabla_h \tilde{q}_h \right) \right] + \nabla_h \cdot \left( \tilde{\psi}_h \nabla_h \tilde{q}_h - \tilde{q}_h \nabla_h \tilde{\psi}_h \right) + \frac{1}{3} \left[ \nabla_h^\perp \tilde{q}_h \cdot \nabla_h \psi_h - \nabla_h^\perp \tilde{\psi}_h \cdot \nabla_h \tilde{q}_h \right].
\]

The expression above replaces the term \( \{ F, H \}_h \) in the formulation of the equation of \( \zeta_h \). The equations for \( \gamma_h \) and \( \phi_h \) remain unchanged. We summarize the full set of equations, for \( \phi_h, \zeta_h \) and \( \gamma_h \), as follows,

\[
(3.74) \quad \begin{cases}
\frac{d}{dt} \phi_i = - \left[ \Delta_h \chi_h \right]_i, \\
\frac{d}{dt} \zeta_i = \frac{1}{6} \left[ \nabla_h \times \left( \tilde{q}_h \nabla_h \psi_h - \tilde{\psi}_h \nabla_h \tilde{q}_h \right) \right] + \nabla_h \cdot \left( \tilde{\psi}_h \nabla_h \tilde{q}_h - \tilde{q}_h \nabla_h \tilde{\psi}_h \right) + \frac{1}{3} \left[ \nabla_h^\perp \tilde{q}_h \cdot \nabla_h \psi_h - \nabla_h^\perp \tilde{\psi}_h \cdot \nabla_h \tilde{q}_h \right] - \left[ \nabla_h \cdot (\tilde{q}_h \nabla_h \chi_h) \right]_i, \\
\frac{d}{dt} \gamma_i = \frac{1}{2} \left[ \nabla_h \times \left( \tilde{q}_h \nabla_h \chi_h \right) \right]_i - \frac{1}{2} \left[ \nabla_h \cdot (\tilde{q}_h \nabla_h \chi_h) \right]_i + \left[ \nabla_h \cdot (\tilde{q}_h \nabla_h \psi_h) \right]_i - \left[ \Delta_h \Phi_h \right]_i - \frac{1}{4 |A_i|} (\tilde{q}_{c_1} (\chi_i - \chi_{i_1}) + \tilde{q}_{c_2} (\chi_{i_2} - \chi_i)).
\end{cases}
\]

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

A discrete analogue of Theorem 2.1 or Theorem 3.1 can also be established.

**Theorem 3.2.** Let \( \phi_h, \zeta_h \), and \( \gamma_h \) be variables that evolve according to equation (3.71). Then an arbitrary functional \( F = F(\phi_h, \zeta_h, \gamma_h) \) of the discrete state variables also evolves according to the equation (3.71).

The proof of this theorem proceeds in a similar way as the proof of Theorem 3.1. We simply points that the new trilinear bracket \( \{ \cdot, \cdot, \cdot \}_h \) will not pose any new difficulty, thanks to the homogeneous Dirichlet boundary conditions assumed on the discrete streamfunction \( \psi_h \).

As a consequence of Theorem 3.2, and thanks to the skew-symmetry property of the discrete Poisson bracket (3.70) (and, indeed, of each of its components), the total energy \( H \) is conserved.

We now examine the conservation of quantities of the form of (3.58). It is clear that the mass (when \( G(q_h) = 1 \)) is conserved under this new scheme. When \( G(q_h) = q_h \), \( C = \int_M \phi_h q_h d\mathbf{x} = \int_M (f + \zeta_h) d\mathbf{x} \) is the circulation. It has functional derivatives

\[
\frac{\delta C}{\delta \phi_h} = 0, \quad \frac{\delta C}{\delta \zeta_i} = 1, \quad \frac{\delta C}{\delta \gamma_h} = 0.
\]
Substituting these functional derivatives into the trilinear bracket (3.69), one has

\[ \{C, H, Z\}_{h,\zeta\zeta\zeta} = \frac{1}{3} \left( \int_M \nabla_h \tilde{H} \cdot \nabla_h \tilde{Z} d\mathbf{x} - \int_M \nabla_h \tilde{Z} \cdot \nabla_h \tilde{H} d\mathbf{x} \right) \]

With the aide of the integration by parts formulas (C.3) and (C.4), and Lemmas C.3 and C.4, one can show that both integrals in the above vanish. It has also been shown in the previous section that both \(\{F, H\}_{h,\gamma\gamma}\) and \(\{F, H\}_{h,\phi\zeta\gamma}\) vanish when \(F\) is taken as the total circulation. Hence the total circulation remains conserved under the new scheme.

When \(G(q_h) = q_h^2/2\), \(C = \int_M \phi_h q_h^2/2 d\mathbf{x}\) is equal to \(Z\), the potential enstrophy. It has been shown in the previous section that both bilinear brackets \(\{F, H\}_{h,\gamma\gamma}\) and \(\{F, H\}_{h,\phi\zeta\gamma}\) vanish when \(F\) is taken as the potential enstrophy. The new trilinear bracket \(\{F, H, Z\}_{h,\zeta\zeta\zeta}\) also vanishes when \(F = Z\), thanks to its skew-symmetry property. Thus, the potential enstrophy is conserved under this new scheme.

4. Linear dispersive analysis. Here we consider an infinite domain with a constant Coriolis force \(f_0\), and no bottom topography (i.e. \(b = 0\)). We also assume that variations in the streamfunction \(\psi_h\) and the velocity potential \(\chi_h\) are small, and that the variations in the fluid thickness \(\phi_h\) is also small compared to its average \(\bar{\phi}\).

Setting \(\hat{\phi}_h = \bar{\phi} + \phi_h'\) in the definition of the geopotential \(\Phi_h\) in (3.2)1 and dropping the quadratic terms, one obtains

\[ \Phi_h = g(\bar{\phi} + \phi_h'). \]

Setting \(\hat{\phi}_h = \bar{\phi} + \phi_h'\) in the last two equations of (3.2), and then dropping the quadratic terms which are small, one obtains

\[ \begin{align*}
\bar{\phi}^{-1} \Delta_h \psi_h &= \zeta_h, \\
\bar{\phi}^{-1} \Delta_h \chi_h &= \gamma_h.
\end{align*} \]

Replacing \(\phi_h\) by \(\bar{\phi} + \phi_h'\) in (3.11), one can also split the PV \(q_h\) into a constant dominant part and a transient part,

\[ q_h = f_0 \bar{\phi} + q_h'. \]

Substituting this expression and (4.1) into (3.41), and again dropping the quadratic nonlinear terms, one obtains

\[ \begin{align*}
\frac{d}{dt} \phi_h' &= -[\Delta_h \chi_h], \\
\frac{d}{dt} \zeta_i &= -\frac{f_0}{\bar{\phi}} \Delta_h \chi_h, \\
\frac{d}{dt} \gamma_h &= \frac{f_0}{\bar{\phi}} \Delta_h \psi_h - g \Delta \phi_h'.
\end{align*} \]
Combining (4.2) with (4.3), one finally obtains the linearized version of the scheme (3.41) as

\[
\begin{align*}
\frac{d}{dt}\phi'_h &= -\bar{\phi}\gamma_h, \\
\frac{d}{dt}\zeta_i &= -f_0\gamma_h, \\
\frac{d}{dt}\gamma_h &= f_0\zeta_h - g\Delta\phi'_h.
\end{align*}
\] (4.4)

The linearized scheme is identical to the Z-grid scheme of [21], which indicates that the scheme (3.41) possess the same dispersive wave relations as the Z-grid scheme.

Analysis on the enstrophy-conserving scheme (3.74) leads to the same conclusion.

5. Conclusion. This work develops conservative finite volume schemes, with optimal dispersive wave relations, for large-scale geophysical flows on unstructured meshes over bounded or unbounded domains. It uses the vorticity-divergence formulation of the dynamical equations for the sake of the dispersive wave relations. The Hamiltonian approach is followed, which seeks to preserve the skew-symmetric structures within the system. Two numerical schemes are developed with the first one conserving the total energy only, and the other slightly more complex one conserving both the energy and (potential) enstrophy. Both schemes are also shown to possess the same optimal dispersive wave relations as those of the Z-grid scheme of [21].

For numerical schemes based on the vorticity-divergence formulations, the issue of boundary conditions is very tricky. For fluid flows, the classical boundary conditions, e.g. the no-flux or no-slip conditions, are typically imposed on the velocity variables, and they have no counterparts for the vorticity/divergence variables. Artificially imposed boundary conditions on the vorticity/divergence can lead to either an under-specified, and over-specified, or an inconsistent system, with serious stability and accuracy implications. Numerous efforts have been spent on this issue ([33, 18, 10]). In this work, the issue of boundary conditions are addressed at three different levels. At the first level, the boundary conditions that are mandated by the analytical system are imposed on the discrete streamfunction and velocity potential directly; see equation (3.6). At the next level, it is made sure that various differential operators are discretized consistently when it comes near the boundary; see (B.4) and (B.6). Lastly, at the highest level on the vorticity and divergence variables, their values on the boundary are not imposed, but are simply evolved along with the other prognostic variables, as dictated by the discrete canonical equations. At this last level, our approach bears some resemblance to, but also substantial difference from that of [3], which adds a prognostic equation for the potential vorticity on the boundary, in addition to the momentum equations in the interior of the domain.

The current work bears the greatest affinity to that of Eldred and Randall ([11]), and that of Bauer and Cotter ([3]). But there are significant differences as well. Both our work and [11] start from the vorticity-divergence formulation and the Hamiltonian approach. But [11] uses the Nambu brackets throughout the whole system to achieve the conservation of enstrophy, and it only considers the global sphere. The current work uses the Nambu bracket only in the $\zeta\zeta$-component of the Poisson bracket, and it takes care of the boundary conditions to ensure that the Poisson/Nambu brackets remain skew-symmetric. The current work share with [3] the common goal of deriving energy and enstrophy conserving schemes over bounded domains. The current work
differs in the discretization methodology (FV vs FEM), the staggering techniques (Z-grid vs C-grid), and the resulting dispersive wave relations (Z-grid vs C-grid).

While the schemes developed in this work are shown to possess excellent conservative properties and dispersive wave relations, other questions regarding accuracy, dynamical behaviors, etc., are left untouched. Also left open are the crucial questions on the real advantages of a doubly-conservative scheme over, say, an energy-conserving only scheme, and how a doubly-conservative scheme should be utilized in practice. These questions will be explored in the second, numerical installment of this project.
Appendix A. Specifications of the mesh.

Fig. A.1. Generic dual meshes, with the domain boundaries passing through the primary cell centers. Left: a generic quadrilateral dual mesh; right: a generic Delaunay-Voronoi dual mesh.

| Set  | Definition                                      |
|------|------------------------------------------------|
| IC   | Set of interior cells                          |
| BC   | Set of boundary cells                          |
| IE   | Set of interior edges                          |
| BE   | Set of boundary edges                          |
| V    | Set of vertices                                |

Our approximation of the function space is based on discrete meshes that consist of polygons. To avoid potential technical issues with the boundary, we shall assume that the domain Ω itself is polygonal. We make use of a pair of staggered meshes, with one called primary and the other called dual. The meshes consist of polygons, called cells, of arbitrary shape, but conforming to the requirements to be specified. The centers of the cells on the primary mesh are the vertices of the cells on the dual mesh, and vice versa. The edges of the primary cells intersect orthogonally with the edges of the dual cells. The line segments of the boundary ∂Ω pass through the centers of the primary cells that border the boundary. Thus the primary cells on the boundary are only partially contained in the domain. Two examples of this mesh type are shown in Figure A.1.

In order to construct function spaces on this type of meshes, some notations are in order, for which we follow the conventions made in [23, 6]. As shown in the diagram in Figure A.2, the primary cells are denoted as \( A_i \), \( 1 \leq i \leq N_c + N_{cb} \), where \( N_c \) denotes the number of cells that are in the interior of the domain, and \( N_{cb} \) the number of cells that are on the boundary. The dual cells, which all lie inside the domain, are denoted as \( A_\nu \), \( 1 \leq \nu \leq N_v \). The area of \( A_i \) (resp. \( A_\nu \)) is denoted as \( |A_i| \) (resp. \( |A_\nu| \)). Each primary cell edge corresponds to a distinct dual cell edge, and vice versa. Thus the primary and dual cell edges share a common index \( e \), \( 1 \leq e \leq N_e + N_{eb} \), where \( N_e \) denotes the number of edge pairs that lie entirely in the interior of the domain, and
Table A.2
Sets of elements defining the connectivity of a unstructured dual grid.

| Set   | Definition                                                                 |
|-------|---------------------------------------------------------------------------|
| $\mathcal{E}C(i)$ | Set of edges defining the boundary of primary cell $A_i$                  |
| $\mathcal{V}C(i)$ | Set of dual cells that form the vertices primary cell $A_i$               |
| $\mathcal{CE}(e)$ | Set of primary cells boarding edge $e$                                    |
| $\mathcal{VE}(e)$ | Set of dual cells boarding edge $e$                                      |
| $\mathcal{CV}(\nu)$ | Set of primary cells that form vertices of dual cell $D_\nu$             |
| $\mathcal{EV}(\nu)$ | Set of edges that define the boundary of dual cell $D_\nu$               |

$N_{cb}$ the number of edge pairs on the boundary, i.e., with dual cell edge aligned with the boundary of the domain. Upon an edge pair $e$, the distance between the two primary cell centers, which is also the length of the corresponding dual cell edge, is denoted as $d_e$, while the distance between the two dual cell centers, which is also the length of the corresponding primary cell edge, is denoted as $l_e$. These two edges form the diagonals of a diamond-shaped region, whose vertices consist of the two neighboring primary cell centers and the two neighboring dual centers. The diamond-shaped region is also indexed by $e$, and will be referred to as $A_e$. The Euler formula for planar graphs states that the number of primary cell centers $N_c + N_{cb}$, the number of vertices (dual cell centers) $N_v$, and the number of primary or dual cell edges $N_e + N_{eb}$ must satisfy the relation

\[(A.1) \quad N_c + N_{eb} + N_v = N_e + N_{eb} + 1.\]
The connectivity information of the unstructured staggered meshes is provided by six sets of elements defined in Table A.2.

For each edge pair, a unit vector \( n_e \), normal to the primary cell edge, is specified. A second unit vector \( t_e \) is defined as

\[
(A.2) \quad t_e = k \times n_e,
\]

with \( k \) standing for the upward unit vector. Thus \( t_e \) is orthogonal to the dual cell edge, but tangent to the primary cell edge, and points to the vertex on the left side of \( n_e \). For each edge \( e \) and for each \( i \in CE(e) \) (the set of cells on edge \( e \), see Table A.2), we define the direction indicator

\[
(A.3) \quad n_{e,i} = \begin{cases} 
1 & \text{if } n_e \text{ points away from primary cell } A_i, \\
-1 & \text{if } n_e \text{ points towards primary cell } A_i,
\end{cases}
\]

and for each \( \nu \in VE(e) \),

\[
(A.4) \quad t_{e,\nu} = \begin{cases} 
1 & \text{if } t_e \text{ points away from dual cell } A_\nu, \\
-1 & \text{if } t_e \text{ points towards dual cell } A_\nu.
\end{cases}
\]

For this study, we make the following regularity assumptions on the meshes. We assume that the diamond-shaped region \( A_e \) is actually convex. In other words, the intersection point of each edge pair falls inside each of the two edges. We also assume that the meshes are quasi-uniform, in the sense that there exists \( h > 0 \) such that, for each edge \( e \),

\[
(A.5) \quad mh \leq l_e, \quad d_e \leq Mh
\]

for some fixed constants \((m, M)\) that are independent of the meshes. The staggered dual meshes are thus designated by \( T_h \). For the convergence analysis, it is assumed in [5] that, for each edge pair \( e \), the primary cell edge nearly bisect the dual cell edge, and miss by at most \( O(h^2) \). This assumption is also made here for the error analysis. Generating meshes conforming to this requirement on irregular domains, i.e. domains with non-smooth boundaries or domains on surfaces, can be a challenge, and will be addressed elsewhere. But we point out that, on regular domains with smooth boundaries, this type of meshes can be generated with little extra effort in addition to the use of standard mesh generators, such as the centroidal Voronoi tessellation algorithm ([7, 8, 9]).

Appendix B. Specifications of the discrete averaging and differential operators.

In this work, a non-accent symbol, such as \( \psi \), usually designates a discrete scalar field defined at the (primal) cell centers, while \( \tilde{\psi} \) on the top, as in \( \tilde{\psi}_h \), designates a discrete scalar field at the vertices, i.e. dual cell centers, and \( \hat{\psi} \) on the top, as in \( \hat{\psi}_h \), designates a discrete scalar field at the edges.

We use \( \overline{\cdot} \) to designate the mappings between primal cell centers and dual cell centers, in both directions. We let \( \psi_h \) be a discrete scalar field defined at cell centers.
Then these mappings can be defined as follows,

(B.1a) \[ \tilde{\psi}_h = \sum_{\nu \in V} \tilde{\psi}_\nu \chi_\nu, \quad \text{with} \quad \tilde{\psi}_\nu = \frac{1}{A_\nu} \sum_{i \in CV(\nu)} \psi_i A_{i,\nu}, \]

(B.1b) \[ \tilde{\psi}_i = \sum_{i \in C} \psi_i \chi_i, \quad \text{with} \quad \psi_i = \frac{1}{2A_i} \sum_{\nu \in VC(i)} \tilde{\psi}_\nu A_{i,\nu}. \]

Generally, on unstructured meshes, the composition of these two mappings is not the identity mapping.

We use \[ \hat{\cdot} \] to designate the mappings between primal cell centers and cell edges, in both directions. Again, with \( \psi_h \) being a discrete scalar field at cell centers, these mappings are specified as follows,

(B.2a) \[ \hat{\psi}_h = \sum_{\nu \in V} \hat{\psi}_e \chi_e, \quad \text{with} \quad \hat{\psi}_e = \frac{1}{1} \sum_{i \in CE(e)} \psi_i, \]

(B.2b) \[ \hat{\psi}_i = \sum_{i \in C} \psi_i \chi_i, \quad \text{with} \quad \psi_i = \frac{1}{2A_i} \sum_{\nu \in VC(i)} \hat{\psi}_\nu A_{i,\nu}. \]

Generally, on unstructured meshes, the composition of these two mappings is not the identity mapping.

The discrete gradient operator \( \nabla_h \) on a cell-centered scalar field \( \psi_h \) is defined as

(B.3) \[ \nabla_h \psi_h = \sum_{e \in E} \nabla_h \psi_h|_e \chi_e \mathbf{n}_e, \quad \text{with} \quad [\nabla_h \psi_h]|_e = -\frac{1}{d_e} \sum_{i \in CE(e)} \psi_i \mathbf{n}_{e,i}. \]

Clearly, \([\nabla_h \psi_h]|_e\) is an approximation of \( \nabla \psi \cdot \mathbf{n} \) at cell edge \( e \). Similarly, the discrete gradient operator \( \nabla_h \) on a triangle-centered scalar field \( \tilde{\psi}_h \) is defined as

(B.4) \[ \nabla_h \tilde{\psi}_h = \sum_{e \in E} \nabla_h \tilde{\psi}_h|_e \chi_e \mathbf{t}_e, \quad \text{with} \quad [\nabla_h \tilde{\psi}_h]|_e = \begin{cases} -\frac{1}{l_e} \sum_{\nu \in VE(e)} \tilde{\psi}_\nu \mathbf{t}_{e,\nu}, & \text{if} \ e \in IE, \\ \frac{t_{e,\nu}(\hat{\psi}_e - \tilde{\psi}_\nu)}{l_e}, & \text{if} \ e \in BE. \end{cases} \]

Clearly, \([\nabla_h \tilde{\psi}_h]|_e\) is an approximation of \( \nabla \tilde{\psi} \cdot \mathbf{t} \) at cell edge \( e \).

The discrete skew gradient operator \( \nabla_h^\perp \) on a cell-centered scalar field \( \psi_h \):

(B.5) \[ \nabla_h^\perp \psi_h = \sum_{e \in E} \nabla_h^\perp \psi_h|_e \mathbf{t}_e, \quad \text{with} \quad [\nabla_h^\perp \psi_h]|_e = -\frac{1}{d_e} \sum_{i \in CE(e)} \psi_i \mathbf{n}_{e,i}. \]

\([\nabla_h^\perp \psi_h]|_e\) is a discretization of \( \nabla^\perp \psi \cdot \mathbf{n} \equiv \partial \psi / \partial n \) at cell edge \( e \).

The discrete skew gradient operator \( \nabla_h^\perp \) on a triangle-centered scalar field \( \tilde{\psi}_h \):

(B.6) \[ \nabla_h^\perp \tilde{\psi}_h = \sum_{e \in E} \nabla_h^\perp \tilde{\psi}_h|_e \chi_e \mathbf{n}_e, \]
with

\[
\left[ \nabla^\perp_h \bar{\psi}_h \right]_e = \begin{cases} 
\frac{1}{l_e} \sum_{\nu \in \mathcal{V}\mathcal{E}(e)} \bar{\psi}_\nu \tau_{e,\nu}, & \text{if } e \in \mathcal{I}\mathcal{E}, \\
\frac{t_{e,\nu}(\bar{\psi}_\nu - \bar{\psi}_e)}{l_e} & \text{for } \nu \in \mathcal{V}\mathcal{E}(e), \text{ if } e \in \mathcal{B}\mathcal{E}.
\end{cases}
\]

where \( \left[ \nabla^\perp_h \bar{\psi}_h \right]_e \) is a discretization of \( \nabla^\perp \psi \cdot \mathbf{n} \equiv -\partial \psi / \partial \tau \) at cell edge \( e \).

We denote by \( u_h \) a discrete vector field that is along the normal direction at each cell edge, and by \( v_h \) a discrete vector field that is along the tangential direction at each cell edge; these discrete vector fields can be expressed as

\[
\begin{align*}
    u_h &= \sum_{e \in \mathcal{E}} u_e \chi_e \mathbf{n}_e, \\
v_h &= \sum_{e \in \mathcal{E}} v_e \chi_e \mathbf{t}_e.
\end{align*}
\]

On these discrete vector fields various discrete differential operators can be defined, using the discrete versions of the divergence theorem or the Green’s theorem.

The discrete divergence operator \( \nabla_h \cdot (\cdot) \) on a discrete normal vector field \( u_h \):

\[
(\text{B.7}) \quad \nabla_h \cdot u_h = \sum_{i \in \mathcal{C}} \left[ \nabla_h \cdot u_h \right]_i \chi_i, \quad \text{with} \quad \left[ \nabla_h \cdot u_h \right]_i = \frac{1}{A_i} \sum_{e \in \mathcal{E}(i)} u_e l_e n_{e,i}.
\]

It is clear that \( \nabla_h \cdot u_h \) is a discrete scalar field on the primal mesh. It is worth noting that, on partial cells on the boundary, the summation on the right-hand side only includes fluxes across the edges that are inside the domain and the partial edges that intersect with the boundary, and this amounts to imposing a no-flux condition across the boundary.

The discrete divergence operator \( \nabla_h \cdot (\cdot) \) on a discrete tangential vector field \( v_h \):

\[
(\text{B.8}) \quad \nabla_h \cdot v_h = \sum_{\nu \in \mathcal{V}} \left[ \nabla_h \cdot v_h \right]_\nu \chi_\nu, \quad \text{with} \quad \left[ \nabla_h \cdot v_h \right]_\nu = \frac{1}{A_\nu} \sum_{e \in \mathcal{E}(\nu)} v_e d_e e_{e,\nu}.
\]

It is clear that \( \nabla_h \cdot v_h \) is a discrete scalar field on the dual mesh.

The discrete curl operator \( \nabla_h \times (\cdot) \) on a discrete normal vector field:

\[
(\text{B.9}) \quad \nabla_h \times u_h = \sum_{\nu \in \mathcal{V}} \left[ \nabla_h \times u_h \right]_\nu \chi_\nu, \quad \text{with} \quad \left[ \nabla_h \times u_h \right]_\nu = -\frac{1}{A_\nu} \sum_{e \in \mathcal{E}(\nu)} u_e e_{e,\nu}.
\]

Thus, the image of the discrete curl operator \( \nabla_h \times (\cdot) \) on each \( u_h \) is a discrete scalar field on the dual mesh.

The discrete curl operator \( \nabla_h \times (\cdot) \) on a discrete tangential vector field:

\[
(\text{B.10}) \quad \nabla_h \times v_h = \sum_{i \in \mathcal{C}} \left[ \nabla_h \times v_h \right]_i \chi_i, \quad \text{with} \quad \left[ \nabla_h \times v_h \right]_i = \frac{1}{A_i} \sum_{e \in \mathcal{E}(i)} v_e l_e n_{e,i}.
\]

Thus, the image of the discrete curl operator \( \nabla_h \times (\cdot) \) on each \( v_h \) is a discrete scalar field on the primal mesh. It is worth noting that, on partial cells on the boundary,
the summation on the right-hand side only includes currents along the edges that are inside the domain and the partial edges that intersect with the boundary, and this amounts to imposing a no-circulation/no-slip condition along the boundary.

For a scalar field $\phi_h$ defined at cell centers, the discrete Laplacian operator $\Delta_h$ can also be defined,

\[(B.11) \quad \Delta_h \phi_h := \nabla_h \cdot (\nabla_h \phi_h) \equiv \nabla_h \times (\nabla_h \phi_h).\]

Appendix C. Discrete vector calculus.

**Lemma C.1.**

\[(C.1) \quad \left( \hat{\psi}_h, \hat{\varphi}_h \right) = \left( \psi_h, \hat{\varphi}_h \right),\]

\[(C.2) \quad \left( \tilde{\psi}_h, \tilde{\varphi}_h \right) = \left( \psi_h, \tilde{\varphi}_h \right).\]

**Proof.** We prove the equality (C.1) first, using the specifications (B.2) for the remapping between center centers and cell edges,

\[
\left( \hat{\psi}_h, \hat{\varphi}_h \right) = \sum_e \left( \frac{1}{2} \sum_{i \in CE(e)} \psi_i \right) \hat{\varphi}_e A_e \\
= \frac{1}{2} \sum_i \psi_i \sum_{e \in CE(i)} \hat{\varphi}_e A_e \\
= \sum_i \psi_i \left( \frac{1}{A_i} \sum_{e \in CE(i)} \hat{\varphi}_e A_e^2 \right) A_i \\
= \left( \psi_h, \hat{\varphi}_h \right).
\]

Similarly, for the equality (C.2), one uses the specifications (B.1), and proceeds,

\[
\left( \tilde{\psi}_h, \tilde{\varphi}_h \right) = \sum_{\nu} \left( \frac{1}{A_{\nu}} \sum_{i \in CV(\nu)} \psi_i A_{i\nu} \right) \tilde{\varphi}_\nu A_\nu \\
= \sum_{\nu} \left( \sum_{i \in CV(\nu)} \psi_i A_{i\nu} \right) \tilde{\varphi}_\nu \\
= \sum_i \psi_i \sum_{\nu \in VC(i)} \tilde{\varphi}_\nu A_{i\nu} \\
= \sum_i \psi_i \left( \frac{1}{A_i} \sum_{\nu \in VC(i)} \tilde{\varphi}_\nu A_{i\nu} \right) A_i \\
= \left( \psi_h, \tilde{\varphi}_h \right).\]

**Lemma C.2.** Let $u_h$ be a discrete normal vector field, $v_h$ a discrete tangential vector field, $\psi_h$ a cell-centered discrete scalar field, and $\tilde{\psi}_h$ a triangle-centered discrete
scalar field. Then the following relations hold,

\begin{align}
(C.3) & \quad (u_h, \nabla_h \psi_h)_{0,h} = -\frac{1}{2} (\nabla_h \cdot u_h, \psi_h)_{0,h}, \\
(C.4) & \quad (u_h, \nabla_h \tilde{\psi}_h)_{0,h} = -\frac{1}{2} \left( \nabla_h \times u_h, \tilde{\psi}_h \right)_{0,h} - \frac{1}{2} \sum_{e \in \mathcal{E}} \tilde{\psi}_e u_e d_e \sum_{\nu \in \mathcal{V}(e)} t_{e,\nu}, \\
(C.5) & \quad (v_h, \nabla_h \tilde{\psi}_h)_{0,h} = -\frac{1}{2} \left( \nabla_h \times v_h, \tilde{\psi}_h \right)_{0,h}, \\
(C.6) & \quad (v_h, \nabla_h \tilde{\psi}_h)_{0,h} = -\frac{1}{2} \left( \nabla_h \cdot v_h, \tilde{\psi}_h \right)_{0,h} + \frac{1}{2} \sum_{e \in \mathcal{E}} \tilde{\psi}_e v_e d_e \sum_{\nu \in \mathcal{V}(e)} t_{e,\nu}.
\end{align}

**Lemma C.3.** Assume that the domain $\mathcal{M}$ is simply connected, and $u_h$ is a discrete normal vector field. Then,

\begin{align}
(C.7) & \quad \nabla_h \cdot u_h = 0 \\
(C.8) & \quad u_h = \nabla_h \tilde{\psi}_h,
\end{align}

if and only if

\begin{align}
(C.9) & \quad \nabla_h \times u_h = 0
\end{align}

for some triangle-centered scalar field $\tilde{\psi}_h$.

**Lemma C.4.** Assume that the domain $\mathcal{M}$ is simply connected, and $u_h$ is a discrete normal vector field. Then,

\begin{align}
(C.10) & \quad u_h = \nabla_h \varphi_h.
\end{align}

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