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Compatible finite element methods for geophysical fluid dynamics

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This article surveys research on the application of compatible finite element methods to large-scale atmosphere and ocean simulation. Compatible finite element methods extend Arakawa's C-grid finite difference scheme to the finite element world. They are constructed from a discrete de Rham complex, which is a sequence of finite element spaces linked by the operators of differential calculus. The use of discrete de Rham complexes to solve partial differential equations is well established, but in this article we focus on the specifics of dynamical cores for simulating weather, oceans and climate. The most important consequence of the discrete de Rham complex is the Hodge–Helmholtz decomposition, which has been used to exclude the possibility of several types of spurious oscillations from linear equations of geophysical flow. This means that compatible finite element spaces provide a useful framework for building dynamical cores. In this article we introduce the main concepts of compatible finite element spaces, and discuss their wave propagation properties. We survey some methods for discretizing the transport terms that arise in dynamical core equation systems, and provide some example discretizations, briefly discussing their iterative solution. Then we focus on the recent use of compatible finite element spaces in designing structure preserving methods, surveying variational discretizations, Poisson bracket discretizations and consistent vorticity transport.

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CONTENTS

1. Introduction

Atmosphere and ocean models used in weather forecasting and climate simulation are built around dynamical cores, which predict the fundamental quantities of fluid motion: fluid velocity, pressure, density, temperature and, in the case of the ocean, salinity. Dynamical cores are computer implementations of numerical discretizations of partial differential equation models of geophysical fluid dynamics in the absence of viscosity. These models are then coupled with physics parametrizations that describe additional physics as well as fluid dynamical processes involving scales that are too small and fast to represent explicitly in the dynamical core. In the case of atmosphere models, this can include radiation processes, cloud models, moisture and precipitation in various phases, models of unresolved convection, boundary layers, and momentum transfer due to unresolved internal waves. In the case of ocean models, this includes vertical mixing due to convection, and parametrization of unresolved eddy motions. Atmosphere and ocean models can be coupled together using parametrizations of air–sea interaction processes, and with other process models to form climate models. Other process models include models of land albedo, land ice, sea ice, atmospheric chemistry, etc. Additionally, in operational forecasting systems, atmosphere and ocean models are blended with observed data using data assimilation algorithms.

A very important aspect of global atmosphere and ocean models is the wide range of timescales. In the rotating compressible Euler equations that model atmospheric flow (although usually with additional approximations), high-frequency motions are possible in the form of pressure waves and internal waves. However, in the solutions relevant to atmosphere models these frequencies are observed to have very low amplitude, with the velocity remaining very close to being horizontal and divergence-free. Since the numerical solution is never anywhere near being

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resolved in an atmosphere model, and due to the coupling with all of the other modelled processes described above, plus the modifications made to the solution by the data assimilation algorithms, it is critically important that unphysical large-amplitude wave motions are avoided. Similar issues arise in the ocean model context. All of this means that it is critically important to pay attention to what happens in the dynamical core at the gridscale, to avoid numerical error triggering these motions. These concerns lie at the heart of the decisions about which discretizations to use in building a dynamical core.

In the past decades, atmosphere and ocean dynamical cores have been mainly built around finite difference, finite volume and pseudospectral methods. In this article we describe a more recent approach to building dynamical cores using compatible finite element methods. Finite element methods have the benefit that they do not depend strongly on the structure of the underlying mesh for their consistency and rate of convergence under mesh refinement. They can use polygonal cells of different types, with triangulations in the horizontal being particularly flexible. This allows mesh refinement in regions of focus, and the construction of meshes that conform to coastlines and areas of high topography curvature. It also allows adaptive mesh refinement, although the advantages of this are less clear in large-scale weather and climate simulation.

The relaxation of mesh structure also allows for more uniform meshes in spherical geometry. Instead of using a latitude–longitude grid, which has very thin cells at the poles due to the convergence of lines of latitude, a cubed sphere mesh (quadrilateral refinement of a cube mapped to a sphere) or an icosahedral mesh (triangular refinement of an icosahedron mapped to a sphere) can be used. These pseudo-uniform grids avoid the parallel scalability bottlenecks (Zängl, Reinert, Rípodas and Baldauf 2015, Adams *et al.* 2019).

Finally, finite element methods allow for increasing the degree of polynomials used in each cell, leading to higher-order accuracy. Higher-order finite element methods have a denser, more structured data layout in each cell, which can be exploited to try to achieve a higher computational intensity, doing more computational work whilst fetching data from nearby cells (Dennis *et al.* 2012, Giraldo, Kelly and Constantinescu 2013).

Compatible finite elements, the subject of this survey, address the problem of spurious numerical waves that cause problems when coupled with numerical errors, physics parametrizations and data assimilation schemes at the gridscale (Staniforth and Thuburn 2012). They can be seen as an extension of the C grid finite difference method (Arakawa and Lamb 1977), which avoids many spurious wave issues when used with quadrilateral cells (and slightly less so with triangular cells). The C grid method achieves this by placing different fields (velocity components, pressure, etc.) on different entities of the grid (cells, edges, vertices) so that the discretized vector calculus operators (div, grad, curl) retain kernels of the appropriate size. This was formalized as the discrete exterior calculus (DEC) (Hirani 2003). Compatible finite element methods do the same thing, but at the level of the finite element

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spaces and the vector calculus mappings between them. These methods have been unified in the finite element exterior calculus (FEEC) (Arnold, Falk and Winther 2006),[1] with a long history going back to the 1970s of applications to porous media, elasticity and fluid dynamics. Their application to geophysical fluid dynamics also has a long history, especially in the ocean (Le Roux, Staniforth and Lin 1998, Walters 2005), and their representation of exact geostrophic balance has been well known from numerical dispersion analysis for some time (Le Roux, Rostand and Pouliot 2007, Rostand and Le Roux 2008). However, it was Cotter and Shipton (2012) who first noticed that it was the compatible structure that was behind this property, and that this structure can be used to understand the numerical dispersion properties of compatible finite element schemes. Following earlier work by the C grid and DEC communities, compatible finite element methods have also been used to build structure preserving discretizations that embed conservation laws at the discrete level.

This article will introduce compatible finite element methods for geophysical fluid dynamics and their properties, and discuss how to build atmosphere and ocean dynamical cores out of them, before focusing on work on structure preserving discretizations. The rest of the article is organized as follows. Section 2 will review compatible finite element spaces and their fundamental properties. Section 3 will discuss their application to linear wave models in geophysical fluid dynamics and the use of the compatible structure to understand discrete wave propagation properties. Moving towards nonlinear dynamical cores, Section 4 will discuss the discretization of transport schemes for compatible finite elements, and Section 5 will use them to describe discretizations for nonlinear geophysical fluid dynamics models and survey their use. One common theme is that the analysis of the convergence and stability of these schemes is very scarce and there is a lot of opportunity for future research in this area. The next four sections concentrate on the use of compatible finite element methods in structure preserving discretizations of various types. Section 6 surveys methods constructed from a discrete Hamilton's principle. Section 7 covers methods constructed from almost-Poisson brackets that ensure conservation of energy and other quantities. Section 8 discusses methods that embed a diagnosed vorticity or potential vorticity field with its own consistent dynamics. Finally, Section 9 discusses some issues common to all structure preserving methods related to non-affine meshes, such as meshes approximating the sphere as well as terrain-following meshes. We then end the survey with a very brief summary in Section 10.

[1] The author uses the term 'compatible finite elements' as a way to discuss them with practitioners when using the language of vector calculus instead of differential forms, which are more unifying but require more background material to discuss.

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2. Compatible finite element spaces

In this section we describe compatible finite element spaces as they are used in geophysical fluid dynamics applications. Compatible finite element spaces are sequences of spaces that form a discrete differential complex (which we shall describe below). In applications to geophysical fluid dynamics, the focus is on the de Rham complex. There is a growing body of work for compatible finite element spaces built around the Stokes complex (e.g. Tai and Winther 2006, Falk and Neilan 2013, Neilan 2020, Hu, Zhang and Zhang 2022), the elasticity complex, and the Regge complex for general relativity (e.g. Christiansen 2011, Christiansen, Gopalakrishnan, Guzmán and Hu 2020), but we shall not discuss those spaces here.

2.1. Preliminary notation

First we establish some notation. Having defined the usual space $L^2(\Omega)$ of square integrable scalar functions on Ω (and writing $L^2(\Omega)^N$ as the space of vector functions on Ω in dimension N), for a domain Ω in three dimensions we have

$$H^1(\Omega) = \{\phi \in L^2(\Omega) \colon \nabla\phi \in L^2(\Omega)\}, \tag{2.1}$$

$$H(\mathrm{curl};\Omega) = \{u \in L^2(\Omega)^3 \colon \nabla \times u \in L^2(\Omega)^3\}, \tag{2.2}$$

$$H(\mathrm{div};\Omega) = u \in L^2(\Omega)^3 \colon \nabla \cdot u \in L^2(\Omega), \tag{2.3}$$

where ∇, $\nabla\cdot$ and $\nabla\times$ are the appropriately defined weak derivative operators; for details, see a textbook on analysis of PDEs (e.g. Evans 2022), or proceed just assuming that these are the usual derivatives for smooth functions and the cellwise derivatives for finite element functions with the appropriate continuity, as we shall discuss below. These spaces are accompanied by norms defined as

$$\|\phi\|^2_{L^2(\Omega)} = \int_\Omega \phi^2 \,\mathrm{d}x, \tag{2.4}$$

$$\|u\|^2_{L^2(\Omega)^N} = \int_\Omega |u|^2 \,\mathrm{d}x, \tag{2.5}$$

$$\|\phi\|^2_{H^1(\Omega)} = \|\phi\|^2_{L^2(\Omega)} + \|\nabla\phi\|^2_{L^2(\Omega)^N}, \tag{2.6}$$

$$\|u\|^2_{H(\mathrm{curl};\Omega)} = \|u\|^2_{L^2(\Omega)^N} + \|\nabla \times u\|^2_{L^2(\Omega)^N}, \tag{2.7}$$

$$\|u\|^2_{H(\mathrm{div};\Omega)} = \|u\|^2_{L^2(\Omega)^N} + \|\nabla \cdot u\|^2_{L^2(\Omega)}. \tag{2.8}$$

In two dimensions, we similarly define

$$H(\mathrm{curl};\Omega) = \{u \in L^2(\Omega)^2 \colon \nabla^\perp \cdot u \in L^2(\Omega)\}, \tag{2.9}$$

$$H(\mathrm{div};\Omega) = \{u \in L^2(\Omega)^2 \colon \nabla \cdot u \in L^2(\Omega)\}, \tag{2.10}$$

having defined the operators $\nabla^\perp\phi = (-\partial_{x_2}\phi, \partial_{x_1}\phi)$ and $\nabla^\perp \cdot u = -\partial_{x_2}u_1 + \partial_{x_1}u_2$. Frequently we drop the Ω from this notation when the meaning is clear. We will

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also use the L^2 inner product notation

$$\langle p, q\rangle = \int_\Omega pq \,\mathrm{d}x \quad \text{for all } p, q \in L^2(\Omega), \tag{2.11}$$

$$\langle u, v\rangle = \int_\Omega u \cdot v \,\mathrm{d}x \quad \text{for all } u, v \in L^2(\Omega)^N, \tag{2.12}$$

noting that

$$\|p\|^2_{L^2(\Omega)} = \langle p, p\rangle, \quad \|u\|^2_{L^2(\Omega)^N} = \langle u, u\rangle. \tag{2.13}$$

We also define $L^2(\Omega)$ inner products for functions on boundaries,

$$\langle\!\langle p, q\rangle\!\rangle = \int_{\partial\Omega} pq \,\mathrm{d}S \quad \text{for all } p, q \in L^2(\partial\Omega), \tag{2.14}$$

$$\langle\!\langle u, v\rangle\!\rangle = \int_{\partial\Omega} u \cdot v \,\mathrm{d}S \quad \text{for all } u, v \in L^2(\partial\Omega)^N. \tag{2.15}$$

2.2. *Discrete de Rham complexes*

In three dimensions, discrete de Rham complexes on a domain Ω consist of subspaces $\mathbb{W}_0 \subset H_1(\Omega)$, $\mathbb{W}_1 \subset H(\mathrm{curl};\Omega)$, $\mathbb{W}_2 \subset H(\mathrm{div};\Omega)$, $\mathbb{W}_3 \subset L^2(\Omega)$, satisfying the following commutation relations:

$$\begin{array}{ccccccc}
\mathbb{W}^0 = H^1 & \xrightarrow{\mathrm{d}^1=\nabla} & \mathbb{W}^1 = H(\mathrm{curl}) & \xrightarrow{\mathrm{d}^2=\nabla\times} & \mathbb{W}^2 = H(\mathrm{div}) & \xrightarrow{\mathrm{d}^3=\nabla\cdot} & L^2 \\
\downarrow \pi_0 & & \downarrow \pi_1 & & \downarrow \pi_2 & & \downarrow \pi_3 \\
\mathbb{W}^0_h & \xrightarrow{\mathrm{d}^1=\nabla} & \mathbb{W}^1_h & \xrightarrow{\mathrm{d}^2=\nabla\times} & \mathbb{W}^2_h & \xrightarrow{\mathrm{d}^3=\nabla\cdot} & \mathbb{W}^3_h,
\end{array} \tag{2.16}$$

where π_i, $i = 0, 1, 2, 3$ are surjective projections, satisfying a bound appropriate to their domain, for example

$$\|\pi_1 u\|_{H(\mathrm{curl})} \leq C\|u\|_{H(\mathrm{curl})} \quad \text{for all } u \in H(\mathrm{curl}). \tag{2.17}$$

The commutation property means that $\mathrm{d}^{k+1}\pi_k u = \pi_{k+1}\,\mathrm{d}^{k+1}u$, $k = 0, 1, 2$. These projection operators (see Arnold *et al.* (2006) for a guide to their construction) do not play a role in computations, but they ensure that the finite element spaces are compatible in the sense that the differential operators ∇, $\nabla\times$ and $\nabla\cdot$ map surjectively onto the kernel of the next operator in the sequence, just as is the case for the infinite-dimensional spaces at the top of the diagram.

In two dimensions, the de Rham complex is shorter, and there are two possible ways to write it:

$$\begin{array}{ccccc}
\mathbb{V}^0 = H^1 & \xrightarrow{\mathrm{d}^1=\nabla^\perp} & \mathbb{V}^1 = H(\mathrm{div}) & \xrightarrow{\mathrm{d}^2=\nabla\cdot} & \mathbb{V}^2 = L^2 \\
\downarrow \pi_0 & & \downarrow \pi_1 & & \downarrow \pi_2 \\
\mathbb{V}^0_h & \xrightarrow{\mathrm{d}^1=\nabla^\perp} & \mathbb{V}^1_h & \xrightarrow{\mathrm{d}^2=\nabla\cdot} & \mathbb{V}^2_h,
\end{array} \tag{2.18}$$

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$$\begin{array}{ccccc} \tilde{\mathbb{V}}^0 = H^1 & \xrightarrow{\mathrm{d}^1=\nabla} & \tilde{\mathbb{V}}^1 = H(\mathrm{curl}) & \xrightarrow{\mathrm{d}^2=\nabla^\perp\cdot} & \tilde{\mathbb{V}}^2 = L^2 \\ \downarrow \pi_0 & & \downarrow \pi_1 & & \downarrow \pi_2 \\ \tilde{\mathbb{V}}^0_h & \xrightarrow{\mathrm{d}^1=\nabla} & \tilde{\mathbb{V}}^1_h & \xrightarrow{\mathrm{d}^2=\nabla^\perp} & \tilde{\mathbb{V}}^2_h. \end{array} \tag{2.19}$$

The equivalence stems from the fact that any vector field in $H(\mathrm{div};\Omega)$ in two dimensions can be transformed into a vector field in $H(\mathrm{curl};\Omega)$ by rotating it by $\pi/2$. In compatible finite element methods for geophysical fluid dynamics we tend to use (2.18), since it allows for local mass conservation and exact application of flux boundary conditions.

2.3. *Discrete Hodge–Helmholtz decomposition*

Crucially for the geophysical fluid dynamics setting, the bounded, commuting, surjective projections ensure a discrete version of the Hodge–Helmholtz decompositions. At the infinite-dimensional level, these decompositions are

$$\mathbb{W}^k = B^k \oplus \mathfrak{h}^k \oplus (B^*)^k, \tag{2.20}$$

where

$$B^k = \{u \in \mathbb{W}^k : \exists \phi \in \mathbb{W}^{k-1}, \text{ with } u = \mathrm{d}^k\phi\}, \tag{2.21}$$

$$\mathfrak{h}^k = \{u \in \mathbb{W}^k : \mathrm{d}^{k+1}u = 0,\ \delta^k u = 0\}, \tag{2.22}$$

$$(B^*)^k = \{u \in \mathbb{W}^k : \exists \phi \in \mathbb{W}^{k+1}, \text{ with } u = \delta^k\phi\}, \tag{2.23}$$

defining the dual operator $\delta^k : \mathbb{W}^k \to \mathbb{W}^{k-1}$ such that

$$\langle \phi, \delta^k u\rangle = -\left\langle \mathrm{d}^{k+1}\phi, u\right\rangle. \tag{2.24}$$

When $u \in \mathbb{W}^k$ is appropriately constructed so that boundary integrals vanish under integration by parts (and sufficiently smooth that integration by parts is well-defined), then we can make the following associations:

$$\delta^0 = -\nabla\cdot, \quad \delta^1 = \nabla\times, \quad \delta^2 = -\nabla. \tag{2.25}$$

For example, considering δ^1, we have

$$\langle v, \delta^1 u\rangle = \langle \nabla \times v, u\rangle = \langle v, \nabla \times u\rangle - \langle\langle v, n \times u\rangle\rangle, \tag{2.26}$$

where n is the outward-pointing normal to $\partial\Omega$. If we choose $u \in \mathring{\mathbb{W}}^2$, where

$$\mathring{\mathbb{W}}^2 = \{u \in \mathbb{W}^2 : u \cdot n = 0 \text{ on } \partial\Omega\}, \tag{2.27}$$

then we obtain that $\delta^1 u = \nabla \times u$ for $u \in \mathring{\mathbb{W}}^2 \cap \mathbb{W}^1$. Similarly, we define

$$\mathring{\mathbb{W}}^0 = \{\phi \in \mathbb{W}^0 : \phi = 0 \text{ on } \partial\Omega\}, \tag{2.28}$$

$$\mathring{\mathbb{W}}^1 = \{u \in \mathbb{W}^1 : u \times n = 0 \text{ on } \partial\Omega\}, \tag{2.29}$$

$$\mathring{\mathbb{W}}^3 = \mathbb{W}^0. \tag{2.30}$$

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See Chapter 3 of Arnold (2018) for an accessible description of the full functional setting for these aspects.

Returning to (2.20), we explain the $\oplus$ notation. It means that any $u \in \mathbb{W}^k$ can be written uniquely as $b + h + c$ with $b \in B^k$, $h \in \mathfrak{h}^k$ and $c \in (B^*)^k$. Further, we have that the spaces B^k, $\mathfrak{h}^k$ and $(B^*)^k$ are mutually orthogonal under the L^2 inner product. When $k = 2$, we recognize this as the Helmholtz decomposition for vector fields, which says that a vector field can be written uniquely as $u = \nabla \times v + h + \nabla\phi$, with $\nabla \cdot h = 0$ and $\nabla \times h = 0$; h is referred to as a 'harmonic vector field'. This decomposition is crucial to the understanding of rapidly rotating fluid dynamics.

As described in Arnold *et al.* (2006), three-dimensional compatible finite element spaces satisfy a discrete Hodge–Helmholtz decomposition,

$$\mathbb{W}_h^k = B_h^k \oplus \mathfrak{h}_h^k \oplus (B^*)_h^k, \tag{2.31}$$

where

$$\mathfrak{h}_h^k = \left\{u \in \mathbb{W}_h^k \colon \mathrm{d}^{k+1}u = 0,\ \delta_h^k u = 0\right\}, \tag{2.32}$$

$$(B^*)_h^k = \left\{u \in \mathbb{W}_h^k \colon \exists \phi \in \mathbb{W}_h^{k+1}, \text{ with } u = \delta_h^k \phi\right\}, \tag{2.33}$$

and we have the discrete dual operator $\delta_h^k \colon \mathbb{W}_h^{k+1} \to \mathbb{W}_h^k$, such that

$$\left\langle \phi, \delta_h^k u \right\rangle = \left\langle \mathrm{d}^{k+1}\phi, u \right\rangle \quad \text{for all } \phi \in \mathbb{W}_h^k,\ u \in \mathbb{W}_h^{k+1}. \tag{2.34}$$

We note the asymmetry under discretization: d^k has the same definition at the discrete level, but δ^k is replaced by the approximation δ_h^k.

The discrete Hodge–Helmholtz decomposition inherits some important properties from the infinite-dimensional decomposition. First, we have $B_h^k \subset B^k$. Second, although $\mathfrak{h}_h^k \neq \mathfrak{h}^k$, we do have that $\dim(\mathfrak{h}_h^k) = \dim(\mathfrak{h}^k)$. Further, $\mathfrak{h}_h^k$ converges to $\mathfrak{h}^k$ as the mesh is refined. These two properties have important consequences for the correct representation of inertial oscillations in geophysical fluid dynamics models. We do not have $(B^*)_h^k \subset (B^*)^k$.

For later discussion we also define

$$\zeta^k = \left\{u \in \mathbb{W}^k \colon d^{k+1}u = 0\right\}, \tag{2.35}$$

noting that $\zeta^k = B^k \oplus \mathfrak{h}^k$. Similarly, we write $\zeta_h^k = B_h^k \oplus \mathfrak{h}_h^k$.

The two-dimensional discrete de Rham complexes also provide an analogous Hodge–Helmholtz decomposition for $\mathbb{V}_h^k$, which is most significant for $\mathbb{V}_h^1$.

2.4. *Two-dimensional compatible finite element spaces used in geophysical fluid dynamics*

For compatible finite element methods for geophysical fluid dynamics, we are mainly focused on the goal of producing three-dimensional fluid models of the atmosphere and ocean. However, model development usually starts by consideration of the rotating shallow water equations, since these equations encompass many of the challenges of designing numerical schemes for atmosphere and ocean

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but without the additional computational challenges of three-dimensional models. On quadrilateral meshes (such as the 'cubed sphere' meshing of the sphere), the most commonly used spaces are $\mathbb{V}_h^0 = Q_k$ (tensor product Lagrange elements, e.g. bilinear, biquadratic), $\mathbb{V}_h^1 = RT_{k-1}$ (Raviart–Thomas elements on quadrilaterals, noting here that we use the traditional numbering convention according to the largest complete polynomial space contained by the finite element, not the UFL/FIAT numbering according to the highest-degree polynomial in the space) and $\mathbb{V}_h^2 = DQ_1$ (discontinuous tensor product Lagrange elements). However, it may be interesting to consider the trimmed serendipity family of elements, especially at higher order (Gillette and Kloefkorn 2019). On triangular meshes (which are much more flexible in allowing local mesh refinement), the main possibilities are $\mathbb{V}_h^0 = P_{k+1}$ (Lagrange elements), $\mathbb{V}_h^1 = BDM_k$ (Brezzi–Douglas–Marini elements on triangles) and $\mathbb{V}_h^2 = DG_{k-1}$, or $\mathbb{V}_h^0 = P_{k+1}$, $\mathbb{V}_h^1 = RT_k$ (Raviart–Thomas elements on triangles) and $\mathbb{V}_h^0 = DG_k$. Whilst in most applications the second grouping is preferred, because it requires fewer degrees of freedom for the same accuracy, in geophysical fluid dynamics this grouping has wave propagation issues related to the Coriolis term, and we tend to prefer the first grouping based on BDM elements (we shall discuss this later). In all of these discrete de Rham complexes, we see the reduction in interelement continuity properties moving across the discrete de Rham complex: $\mathbb{V}_h^0$ contains only continuous functions, $\mathbb{V}_h^1$ requires continuity of normal components of its vector-valued functions across cell facets (but not tangential components) and $\mathbb{V}_h^2$ has functions with no interelement continuity constraints. See Boffi, Brezzi and Fortin (2013) for definitions of the finite elements introduced in this paragraph.

2.5. *Three-dimensional compatible finite element spaces used in geophysical fluid dynamics*

When moving to three-dimensional models, since the Earth's atmosphere and ocean are much larger in horizontal extent than the vertical, good preservation of hydrostatic balance (balance between gravitational acceleration and vertical pressure gradient) requires the use of prismatic meshes that are constructed by extruding a two-dimensional base mesh into layers. When the base mesh is constructed from quadrilaterals, this produces hexahedra, and when the base mesh is constructed from triangles, this produces triangular prisms. Three-dimensional discrete de Rham complexes are constructed on these spaces by a tensor product of a two-dimensional de Rham complex on the base mesh with a one-dimensional de Rham complex for the vertical direction, given by

$$\begin{array}{ccc} \mathbb{U}^0 = H^1 & \xrightarrow{\mathrm{d}^1=\partial_x} & \mathbb{V}^1 = L^2 \\ \downarrow \pi_0 & & \downarrow \pi_1 \\ \mathbb{U}_h^0 & \xrightarrow{\mathrm{d}^1=\partial_x} & \mathbb{U}_h^1. \end{array} \tag{2.36}$$

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Excluding splines, etc., the main family of options for these one-dimensional spaces is continuous Lagrange elements of degree $k+1$ for $\mathbb{U}^0_h$ and discontinuous Lagrange elements of degree k for $\mathbb{U}^1_h$. The three-dimensional discrete de Rham complex is then formed on the reference cell $\hat{K}_3 = \hat{K}_2 \times \hat{K}_1$ as follows:

$$\mathbb{W}^0_h(\hat{K}_3) = \mathbb{V}^0_h(\hat{K}_2) \otimes \mathbb{U}^0_h(\hat{K}_1), \tag{2.37}$$

$$\mathbb{W}^1_h(\hat{K}_3) = \underbrace{\hat{k}\mathbb{V}^0_h(\hat{K}_2) \otimes \mathbb{U}^1_h(\hat{K}_1)}_{=\mathbb{W}^{1,V}_h} \oplus \underbrace{\iota(\mathbb{V}^1_h(\hat{K}_2))^{\perp} \otimes \mathbb{U}^0_h(\hat{K}_1)}_{=\mathbb{W}^{1,H}_h}, \tag{2.38}$$

$$\mathbb{W}^2_h(\hat{K}_3) = \underbrace{\mathbb{V}^2_h(\hat{K}_2) \otimes \hat{k}\mathbb{U}^0_h(\hat{K}_1)}_{=\mathbb{W}^{2,V}_h} \oplus \underbrace{\iota(\mathbb{V}^1_h(\hat{K}_2)) \otimes \mathbb{U}^1_h(\hat{K}_1)}_{=\mathbb{W}^{2,H}_h}, \tag{2.39}$$

$$\mathbb{W}^3_h(\hat{K}_3) = \mathbb{V}^2_h(\hat{K}_2) \otimes \mathbb{U}^1_h(\hat{K}_1). \tag{2.40}$$

Here we write coordinates on $\hat{K}_3$ as (x, z) with $x \in \hat{K}_2$ and $z \in \hat{K}_1$, defining the tensor product $V(K_2)\otimes U(K_1)$ as the span of function products $u(x)v(z)$ with $u \in V(K_2)$ and $v \in V(K_1)$. Further, $\hat{k}$ is the unit upward-pointing vector, ι is the inclusion operator that maps two-dimensional vectors into equivalent three-dimensional vectors with zero vertical part, and $\perp$ is the operator that rotates vectors by a quarter of a rotation in the horizontal direction. These latter technicalities involving ι, $\hat{k}$ and $\perp$ can all be avoided in the unified presentation of spaces of discrete differential forms in the finite element exterior calculus, which also unifies many other aspects across dimensions, numbering of the spaces, etc. See Arnold and Awanou (2014) for a full presentation of tensor product discrete differential forms.

Again, in all of these three-dimensional discrete de Rham complexes we see the reduction in interelement continuity properties moving across the discrete de Rham complex: $\mathbb{W}^0_h$ contains only continuous functions, $\mathbb{W}^1_h$ requires continuity of tangential components of its vector-valued functions across cell facets (but not normal components), $\mathbb{W}^2_h$ requires continuity of normal components of its vector-valued functions across cell facets (but not tangential components) and $\mathbb{W}^3_h$ has functions with no interelement continuity constraints.

As indicated in (2.38)–(2.39). the $\mathbb{W}^1_h$ and $\mathbb{W}^2_h$ spaces can be split into vertical and horizontal parts, indicated by the V and H superscripts, respectively. As suggested by this notation, the vertical part contains vector fields that point in the vertical direction, whilst the horizontal part contains vector fields that point in the horizontal direction. After Piola transformation to mesh cells (discussed in Section 2.6), this decomposition is not preserved in general. However, if mesh cells are arranged into a global tensor product mesh (i.e. flat vertical layers), then this decomposition is preserved. This will also occur in a spherical annulus meshed by radially extruding a two-dimensional surface mesh of the sphere (or an approximation of one). If a terrain-following mesh is used, so that the side walls of the mesh are arranged vertically but the horizontal layers move up and down

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to conform to mountain ranges on the surface, the decomposition is only partially preserved: $\mathbb{W}_h^{1,H}$ remains tangential to the 'up' direction and $\mathbb{W}_h^{2,V}$ remains normal to the 'up' direction, but $\mathbb{W}_v^{1,V}$ will contain some horizontal component and $\mathbb{W}_h^{2,V}$ will contain some vertical component.

In discretizations for geophysical fluid dynamics it is important that the gravity term can be balanced by a vertical pressure gradient. To avoid degeneracy in this balance, discussed in Section 3.8, it is necessary to use a finite element space $\mathbb{W}_\theta$ for temperature variables (entropy, temperature, potential temperature, etc.) that is adapted to the vertical part of $\mathbb{W}_h^2$, which is used to represent the velocity in this framework. We choose $\mathbb{W}^\theta(\hat{K})$ so that $\theta \in \mathbb{W}^\theta(\hat{K}) \implies \hat{k}\theta \in \mathbb{W}_h^{2,V}(\hat{K})$, that is,

$$\mathbb{W}_\theta(\hat{K}) = \mathbb{V}_h^0(\hat{K}_2) \otimes \mathbb{U}_h^1(\hat{K}_1). \tag{2.41}$$

It is also useful to construct vertical slice models by making analogous tensor product constructions combining the $(\mathbb{U}_h^0, \mathbb{U}_h^1)$ de Rham complex with itself. Since the only possible one-dimensional meshes are intervals, this just leads to the usual tensor product elements for quadrilaterals that we have already discussed above.

For further description of the construction and efficient implementation of these tensor product elements within an automated system, see McRae *et al.* (2016). The use of extruded meshes also has computational benefits that offset the additional computational cost of using unstructured meshes in the horizontal. If a semistructured data layout is used (i.e. a horizontal unstructured index and a vertical structured one), then for a reasonable number of vertical layers (20 is already enough in numerical experiments) the lookups to find data in the unstructured grid data structure are negligible compared to the computational work done on data loaded into memory. Thus there is no significant performance penalty to using an unstructured data structure in the horizontal (Bercea *et al.* 2016). This means that the benefits of the flexibility and mesh invariance of the unstructured grid data structure in the horizontal can be exploited in performant three-dimensional geophysical fluid models.

2.6. *Local to global mappings*

Whilst there has been work on, for example, $H(\mathrm{div})$ elements on quadrilaterals where the polynomials are defined directly on the mesh elements (Arbogast and Correa 2016), here we mostly restrict discussion to discrete de Rham complexes that are constructed on reference elements and mapped to mesh elements using Piola maps. In three dimensions, this corresponds to the following set of relations:

$$\psi \in \mathbb{W}_h^0(K) \colon \psi \circ g_K = \hat{\psi},\ \hat{\psi} \in \mathbb{W}_h^0(\hat{K}), \tag{2.42}$$

$$u \in \mathbb{W}_h^1(K) \colon u \circ g_K = J^{-\top}\hat{u},\ \hat{u} \in \mathbb{W}_h^1(\hat{K}), \tag{2.43}$$

$$w \in \mathbb{W}_h^2(K) \colon u \circ g_K = J\hat{w}/\det J,\ \hat{w} \in \mathbb{W}_h^2(\hat{K}), \tag{2.44}$$

$$\phi \in \mathbb{W}_h^3(K) \colon \phi \circ g_K = \hat{\phi}/\det J,\ \hat{\phi} \in \mathbb{W}_h^3(\hat{K}), \tag{2.45}$$

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where g_K is the map between reference cell $\hat{K}$ and mesh cell K, with derivative J, $J^{-\top}$ means the inverse of the transpose of J, and $\circ$ indicates function composition, that is, $f \circ g$ is another function with $(f \circ g)(x) = f(g(x))$. This ensures that the discrete de Rham complex property is preserved under the mapping from $\hat{K}$ to K. To define $\mathbb{W}_\theta(\Omega)$, we just use straightforward composition with the reference to cell map as is done for $\mathbb{W}_h^0$. This leads to some differences between $\mathbb{W}_h^\theta$ and the vertical component of $\mathbb{W}_h^2(\Omega)$ when terrain-following coordinates are used.

In two dimensions when using (2.18), this becomes

$$\psi \in \mathbb{V}_h^0(K) \colon \psi \circ g_K = \hat{\psi},\ \hat{\psi} \in \mathbb{V}_h^0(\hat{K}), \tag{2.46}$$

$$w \in \mathbb{V}_h^1(K) \colon u \circ g_K = J\hat{w}/\det J,\ \hat{w} \in \mathbb{V}_h^1(\hat{K}), \tag{2.47}$$

$$\phi \in \mathbb{V}_h^2(K) \colon \phi \circ g_K = \hat{\phi}/\det J,\ \hat{\phi} \in \mathbb{V}_h^2(\hat{K}). \tag{2.48}$$

In geophysical fluid dynamics applications, being able to solve equations on the surface of a sphere is important. In general, two-dimensional complexes can be extended to orientable manifolds embedded in three dimensions by restricting vector fields to be tangential to the manifold at each point. Then, for such a vector field u, we define $u^\perp = k \times u$, $\nabla^\perp u = k \times \nabla u$ and $\nabla^\perp \cdot u = k \cdot \nabla \times u$, where ∇ is now the projection of the gradient onto the tangent plane. In fact, these operations can all be given intrinsic definitions on any two-dimensional manifold without reference to an external space $\mathbb{R}^3$ containing the manifold, best expressed using the language of differential forms. However, we do not do this here; see Arnold *et al.* (2006) for intrinsic constructions using differential forms.

The geometric factors in these formulae introduce complications. These are related both to the approximation properties of the spaces and to their computer implementation, the latter due to the resulting non-polynomial integrands in weak formulations. When g_K is an affine transformation, J is constant on each cell, and no alterations to the approximation properties arise. However, when g_K is non-affine, J is non-constant. This means that the transformed basis functions may not span the same polynomial spaces as they do on the reference cell. Arnold, Boffi and Falk (2005) and Falk, Gatto and Monk (2011) showed that this occurs for transformed $H(\mathrm{div})$ and $H(\mathrm{curl})$ elements on non-affine quadrilaterals and hexahedra. This interferes with the standard approximation theory error estimates, because they apply the Bramble–Hilbert lemma considering the largest polynomial space spanned by the basis. The degradation of approximation theory was demonstrated in practice in those papers. This presents a concern for the applicability of these spaces in geophysical fluid dynamics, because we encounter non-affine transformations when using quadrilaterals or higher-order triangular cells (i.e. triangles that have been curved to better approximate the sphere) to approximate the surface of the sphere. These spaces are also used when extruding the sphere radially to make a spherical annulus, required for three-dimensional atmosphere and ocean models; this leads to non-affine prismatic meshes. Non-affine cells also arise when terrain-following meshes are used. These are meshes that slope layers up and down to conform to

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mountain ranges at the Earth's surface in the atmosphere and ocean. Fortunately, these approximation issues can be avoided through the framework of Holst and Stern (2012), who used Strang-type estimates to consider the 'variational crime' of a sequence of meshes that only conform to a manifold in the limit. Provided that the meshes can be obtained by piecewise smooth mappings from an affine mesh (i.e. a mesh consisting of cells mapped to the reference cell by affine transformations), then approximation error bounds can be obtained that match those of the reference cell. For meshes of interest in geophysical fluid dynamics, this covers the sphere meshes described above, as well as terrain-following meshes obtained by smooth transformation (smoothing of topography is standard practice in atmosphere and ocean modelling). For the case of meshes (non-affine or otherwise) of the sphere extruded into a spherical annulus, Natale, Shipton and Cotter (2016) showed that these meshes can be obtained via transformation from an affine mesh embedded in four dimensions.

Additionally, on unstructured meshes one must take care that the degrees of freedom are correctly matched up on facets, and with the correct sign (since they involve normal and tangential components in general). A systematic approach for this was set out by Rognes, Kirby and Logg (2010), which is now implemented in a number of finite element software systems, such as FEnICS (Logg, Mardal and Wells 2012) and Firedrake (Rathgeber *et al.* 2016). Such systems are very useful as an aid to productivity when dealing with the complexities of compatible finite elements.

2.7. *Replacing* $\nabla\cdot$ *with* DIV

One practical modification to this framework on non-affine meshes is to replace the transformation for the L^2 space ($V = \mathbb{V}_h^2$ in two dimensions or $V = \mathbb{W}_h^3$ in three dimensions) with straightforward composition, that is,

$$\phi \in V(K)\colon \phi \circ g_K = \hat{\phi},\ \hat{\phi} \in V(\hat{K}). \tag{2.49}$$

Then the discrete de Rham complex can be restored by replacing $\nabla\cdot$ with DIV $:= P_V \nabla\cdot$, where P_V is the L^2 projection into V. This is always a local operation since V is a discontinuous space with no interelement coupling. The diagram still commutes, since if $u \in H(\mathrm{div}; \Omega)$ then $\pi_N \circ \nabla\cdot = \mathrm{DIV}$. This idea was originally proposed in Bochev and Ridzal (2009), who defined DIV equivalently in the case of RT_0 spaces on quadrilateral grids using the discrete exterior calculus framework by evaluating fluxes through edges, after which the definition as projection of the divergence can be obtained using the divergence theorem. The extension to more general $H(\mathrm{div})$ finite element spaces on non-affine meshes was probably clear to those authors, but it was also discussed from a practical perspective in Shipton, Gibson and Cotter (2018).

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2.8. *Primal–dual grids*

There have been various attempts to build complementary spaces on dual grids, in order to avoid the global mass solves that are required to compute δ. These spaces are linked by 'discrete Hodge star' operators ($\star_0, \star_1, \star_2$), with mappings indicated in the following diagram:

$$\begin{array}{ccccc} \mathbb{V}_h^0 & \xrightarrow{\mathrm{d}^1=\nabla^\perp} & \mathbb{V}_h^1 & \xrightarrow{\mathrm{d}^2=\nabla\cdot} & \mathbb{V}_h^2, \\ \downarrow \star_0 & & \downarrow \star_1 & & \downarrow \star_2 \\ \tilde{\mathbb{V}}_h^2 & \xleftarrow{\mathrm{d}^2=\nabla^\perp\cdot} & \tilde{\mathbb{V}}_h^1 & \xleftarrow{\mathrm{d}^1=\nabla} & \tilde{\mathbb{V}}_h^0. \end{array} \tag{2.50}$$

It is important that the discrete Hodge star maps are invertible. The approach is clearest for lowest-order spaces, where there is at most one nodal degree of freedom per edge, vertex or cell in the definition of each space, in analogy with the discrete exterior calculus (Hirani 2003). Thuburn and Cotter (2015) and Melvin and Thuburn (2017) constructed complementary spaces on triangulations and their duals by subdividing cells into triangles and placing RT_0 elements in each subcell. A constraint is applied so that the d_2 operators produce constant functions over the primal and dual cells, respectively. This scheme produces an extension of the primal–dual finite difference C grid approach to the consistent finite element setting; inconsistencies in the Coriolis term occur on dual icosahedral and cubed sphere set-ups in the framework of Thuburn and Cotter (2012) and Thuburn, Cotter and Dubos (2014*a*). The framework of mimetic spectral elements extends this idea to higher-order polynomial spaces (Lee, Palha and Gerritsma 2018).

3. Wave propagation properties

In this section we review the properties of compatible finite element discretizations applied to linearized geophysical fluid dynamics. We will see the favourable properties of the C grid finite difference approach to finite element methods. It is these properties that underpin the Met Office's choice to use compatible finite element methods to build their 'GungHo' atmospheric dynamical core that lies at the centre of their next generation LFRic modelling system (e.g. Adams *et al.* 2019).

3.1. *Compatible discretization of the linear rotating shallow water equations*

For now, we consider compatible finite element methods applied to the linearized rotating shallow water equations on the doubly periodic plane with constant Coriolis parameter,

$$u_t + \underbrace{fu^\perp}_{\text{Coriolis}} + \underbrace{g\nabla\eta}_{\text{pressure gradient}} = 0, \; \eta_t + H\nabla\cdot u = 0, \tag{3.1}$$

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where u is the horizontal velocity, $h = \eta + H$ is the layer height with H constant and η integrating to zero, f is the (constant) Coriolis parameter and g is the acceleration due to gravity. The $\perp$ operator rotates vectors one quarter of a rotation, to obtain $u^\perp = (-u_2, u_1)$. These equations are solved in two dimensions.

We use the Helmholtz decomposition $u = \nabla^\perp\psi + \bar{u} + \nabla\phi$, where $\bar{u}$ is a spatially constant (but possibly time-dependent) vector field, as the harmonic vector fields in the doubly periodic plane are of this form. Then we may write

$$\phi_t - f\psi + g\eta = 0, \tag{3.2}$$

$$\psi_t + f\phi = 0, \tag{3.3}$$

$$\bar{u}_t + f\bar{u}^\perp = 0, \tag{3.4}$$

$$\eta_t + H\nabla^2\phi = 0. \tag{3.5}$$

First, we observe that the harmonic component $\bar{u}$ is decoupled and rotates at frequency f. These are called inertial oscillations. Second, we can find steady solutions with $\phi = 0$, $\bar{u} = 0$, $\psi = g\eta/f$. These solutions correspond to states of 'geostrophic balance', where the velocity is divergence-free and the pressure gradient term cancels out the Coriolis term. The remaining solutions are inertia–gravity waves with ϕ non-zero. Applying time derivatives to (3.5) and (3.2), we eliminate ψ and η (by also using (3.3)), to obtain

$$\phi_{tt} + f^2\phi - gH\nabla^2\phi = 0, \tag{3.6}$$

which is the inertia–gravity wave equation. When $f = 0$, this becomes the wave equation with wavespeed $\sqrt{gH}$. When $f \neq 0$ (a positive sign would be used for Northern Hemisphere dynamics) then the equation becomes a Klein–Gordon equation, which is dispersive.

Numerically induced oscillations (physical and spurious) in shallow water models have been extensively examined by Le Roux in a series of papers using dispersion analysis (Le Roux *et al.* 2007, Le Roux and Pouliot 2008, Rostand and Le Roux 2008, Le Roux 2012), including for discretizations in the compatible finite element family. Much of the vocabulary we use in this section has been taken from that work.

To discretize this equation in space using compatible finite elements, we pick a two-dimensional discrete de Rham complex $(\mathbb{V}_h^0, \mathbb{V}_h^1, \mathbb{V}_h^2)$, and choose $u \in \mathbb{V}_h^1$, $\eta \in \mathbb{V}_h^2$. Then the usual introduction of inner products with test functions and integration by parts leads to the discrete formulation

$$\langle w, u_t\rangle + \langle w, fu^\perp\rangle - \langle \nabla\cdot w, g\eta\rangle = 0 \quad \text{for all } w \in \mathbb{V}_h^1, \tag{3.7}$$

$$\langle \alpha, \eta_t + H\nabla\cdot u\rangle = 0 \quad \text{for all } \alpha \in \mathbb{V}_h^2. \tag{3.8}$$

Since $\eta_t + H\nabla\cdot u \in \mathbb{V}_h^2$, we may choose $\alpha = \eta_t + H\nabla\cdot u$ in (3.8), concluding that

$$\eta_t + H\nabla\cdot u = 0 \quad \text{in } L^2(\Omega). \tag{3.9}$$

This is a useful property that we will use later.

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3.2. Geostrophic balance

In large-scale atmosphere and ocean applications, it is very important that discretizations can preserve states of geostrophic balance well; this is usually tested on the linear rotating shallow water equations as discussed here. Cotter and Shipton (2012) proved that compatible finite element discretizations will have exactly steady geostrophic balanced solutions. To be precise, for any divergence-free velocity field u with zero harmonic component $\bar{u}$, there exists an η such that (u, η) form a steady solution in geostrophic balance. To show this, we just find $\psi \in \mathbb{V}_h^0$ such that $u = \nabla^\perp \psi$ (possible from the discrete Helmholtz decomposition), and pick η as the L^2 projection of ψ into $\mathbb{V}_2$ before multiplying by g/f. Then

$$\langle \nabla \cdot w, g\eta \rangle = \langle \nabla \cdot w, f\psi \rangle = -\langle w, f\nabla\psi \rangle = \langle w, fu^\perp \rangle \quad \text{for all } w \in \mathbb{V}_h^1, \tag{3.10}$$

where the first equality holds from the projection, since $\nabla \cdot w \in \mathbb{V}_h^2$. The second equality holds by integration by parts, which is exact because $w \in H(\mathrm{div})$ and $\psi \in H^1$. The final equality follows from $u = \nabla^\perp \psi$.

What is not true is that for every η there exists a ψ giving a steady-state solution. This is because the L^2 projection from $\mathbb{V}_h^0$ to $\mathbb{V}_h^2$ is not a bijection. However, this does not hold in the C grid finite difference case either.

It is also important that discretizations correctly represent inertial oscillations. In the linear rotating shallow water equations, the only solutions with $\eta = 0$ are the inertial oscillations with spatially constant $u = \bar{u}$ rotating at frequency f. It is important that discretizations are free of spurious additional inertial modes, i.e. solutions with $\eta = 0$ but with spatially varying u. Le Roux (2012) examined spurious modes in various finite element discretizations, showing that when they are present they lead to degraded error convergence rates. They have also been observed to lead to problems in practical ocean model simulations, where they can be excited by nonlinearity in baroclinic jets. This results in the formation of spurious grid-scale oscillatory patterns that do not change the pressure/layer depth (Danilov and Kutsenko 2019). In a closed bounded domain with boundary condition $u \cdot n = 0$, we do not expect inertial oscillations because the space of harmonic vector fields only contains 0. However, it is possible for spurious inertial oscillations to satisfy the boundary condition, leading to their excitation.

3.3. Inertial oscillations

Natale *et al.* (2016) showed that compatible finite element discretizations applied to the rotating shallow water equations in the periodic plane have the following property: the only time-varying solutions of (3.7)–(3.8) with $\eta = 0$ have spatially constant u_t, corresponding to inertial oscillations oscillating with frequency f. Any time-independent solutions are in the kernel of the discrete Coriolis operator, i.e. $u \in \mathbb{V}_h^1$ such that

$$\langle w, u^\perp \rangle = 0 \quad \text{for all } w \in \mathbb{V}_h^1. \tag{3.11}$$

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In other words, these discretizations are free from inertial oscillations. To see this, first note that if $\eta = 0$, then (3.9) implies that $\nabla \cdot u = 0$, so that $u = k + \nabla^\perp \psi$ for $k \in \mathfrak{h}_h$ and $\psi \in \mathbb{V}_h^0$, from the discrete Helmholtz decomposition. Using $w = \nabla^\perp \gamma$ in (3.7), we get

$$\langle \nabla^\perp \gamma, u_t \rangle = -f \langle \nabla^\perp \gamma, u^\perp \rangle = f \langle \gamma, \nabla \cdot u \rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}_h^0. \tag{3.12}$$

Hence u_t is orthogonal to B_h^k, i.e. $u_t \in \mathfrak{h}_h$. We know from the discrete Hodge–Helmholtz decomposition that $\dim(\mathfrak{h}_h) = \dim(\mathfrak{h}) = 2$ on the periodic plane; $\mathfrak{h}$ is the set of constant vector fields. In fact, since the constant vector fields are in $\mathbb{V}_h^1$, they are divergence-free and in the kernel of δ_h. Time-independent divergence-free solutions satisfy

$$0 = \langle w, u_t \rangle = -f \langle w, u^\perp \rangle \quad \text{for all } w \in \mathbb{V}_h^1, \tag{3.13}$$

that is, they are in the kernel of the discrete Coriolis operator. Vector fields in this kernel are referred to as 'Coriolis modes'. They are the main downside of compatible discretizations, but the dimension of this kernel is always found to be finite and resolution-independent in analyses by Rostand and Le Roux (2008); in fact this number is typically very small. These Coriolis modes are also always found in C grid finite difference discretizations.

3.4. *Inertia gravity waves*

Cotter and Shipton (2012) also examined the discrete inertia–gravity waves that correspond to solutions of the Klein–Gordon equation above. Writing $u = \nabla^\perp \psi + \delta \phi$ for $\psi \in \mathbb{V}_0$ and $\phi \in \mathbb{V}_2$ (having already discarded the harmonic component since it decouples), and choosing both $w = \nabla^\perp \gamma$ for $\gamma \in \mathbb{V}_h^0$ and $w = \delta \alpha$ for $\alpha \in \mathbb{V}_h^2$, we obtain

$$\langle \delta \alpha, \delta \phi_t \rangle - f \langle \delta \alpha, \nabla \psi \rangle - g \langle \delta \alpha, \delta \eta \rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}_2, \tag{3.14}$$

$$\langle \nabla \gamma, \nabla \psi_t \rangle + f \langle \nabla \gamma, \delta \phi \rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}_h^0, \tag{3.15}$$

$$\langle \phi, \eta_t + H \nabla \cdot \delta \phi \rangle = 0 \quad \text{for all } \phi \in \mathbb{V}_h^2. \tag{3.16}$$

Using the definition of δ, and the fact that the height equation holds in L^2, we get

$$-\langle \alpha, \nabla \cdot \delta \phi_t \rangle + f \left\langle \alpha, \nabla^2 \psi \right\rangle + g \langle \alpha, \nabla \cdot \delta \eta \rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}_2, \tag{3.17}$$

$$\langle \nabla \gamma, \nabla \psi_t \rangle - f \langle \gamma, \nabla \cdot \delta \phi \rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}_h^0, \tag{3.18}$$

$$\eta_t + H \nabla \cdot \delta \phi = 0. \tag{3.19}$$

We can recognize the operator $\nabla \cdot \delta$ as the mixed approximation $\tilde{\nabla}^2$ of the Laplacian defined by

$$\left\langle \alpha, \tilde{\nabla}^2 \phi \right\rangle - \langle \alpha, \nabla \cdot \sigma \rangle = 0 \quad \text{for all } \alpha \in \mathbb{V}_h^2. \tag{3.20}$$

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After restricting to $\overline{\mathbb{V}}^2_h$, defined by

$$\overline{\mathbb{V}}^2_h = \left\{ \phi \in \mathbb{V}^2_h : \int_\Omega \phi \, \mathrm{d}x = 0 \right\}, \tag{3.21}$$

this discretization is well known to be invertible, stable and convergent. Hence, when $f = 0$, we can deduce

$$\phi_{tt} - gH\tilde{\nabla}^2\phi = 0, \tag{3.22}$$

i.e. the mixed approximation of the wave equation for $\phi \in \overline{\mathbb{V}}^2_h$.

When $f \neq 0$, we have to introduce projection operators

$$P_0 : \overline{\mathbb{V}}^2_h \to \overline{\mathbb{V}}^0_h, \quad P_2 : \overline{\mathbb{V}}^0_h \to \overline{\mathbb{V}}^2_h, \tag{3.23}$$

defined by

$$\langle \nabla\gamma, \nabla P_0\phi \rangle = \langle \nabla\gamma, \delta\phi \rangle \quad \text{for all } \gamma \in \overline{\mathbb{V}}^0_h, \tag{3.24}$$

$$\left\langle \alpha, -\tilde{\nabla}^2 P_2\psi \right\rangle := \langle \delta\alpha, \delta P_2\psi \rangle = \langle \delta\alpha, \nabla\phi \rangle \quad \text{for all } \gamma \in \overline{\mathbb{V}}^2_h. \tag{3.25}$$

P_0 is well-posed since it just involves solving the usual Galerkin discretization of the Laplacian on $\overline{\mathbb{V}}^0_h$, whilst P_2 is well-posed since it involves solving the mixed discretization as we have already discussed.

Using P_0 and P_2, we get

$$\phi_t - fP_2\psi + gh = 0, \tag{3.26}$$

$$\psi_t + fP_0\phi = 0, \tag{3.27}$$

$$\eta_t + H\tilde{\nabla}^2\phi = 0, \tag{3.28}$$

from which we can deduce the discrete Klein–Gordon equation

$$\phi_{tt} + f^2 P_2 P_0 \phi - gH\tilde{\nabla}^2\phi = 0. \tag{3.29}$$

The behaviour of the numerical dispersion relation depends on the kernel of the composition P_2P_0, for which a lower bound is obtained by considering the relative sizes of $\bar{\mathbb{V}}^0_h$ and $\bar{\mathbb{V}}^2_h$. For RT_k on quadrilaterals, these two spaces have the same dimension in the periodic domain, so this projection is not too harmful. For RT_k spaces on triangles, $\dim(\bar{\mathbb{V}}_2) > \dim(\bar{\mathbb{V}}_0)$, so P_2P_0 is not surjective. In the case of the C grid finite difference method on triangles, a similar issue arises, causing high- and low-frequency branches of the numerical dispersion relation to intertangle, leading to numerical noise when f is sufficiently large (Danilov 2010). Further analysis is required to really pin down these issues in the compatible finite element case. For BDM_k spaces on triangles, we have the opposite situation, $\dim(\bar{\mathbb{V}}_2) < \dim(\bar{\mathbb{V}}_0)$, so there is at least the chance for P_2P_0 to be surjective (although both projection operators will have checkerboard modes in their kernel on structured meshes). This suggests that BDM spaces are more appropriate for

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geophysical fluid dynamics using triangular meshes, but further analysis of these issues is needed to make these statements more precise.

3.5. *Spectral gaps and zero group velocity*

Staniforth, Melvin and Cotter (2013) and Melvin, Staniforth and Cotter (2014) examined the numerical dispersion relation for the cases of RT_0 and RT_1 on quadrilaterals, motivated by building discretizations on the sphere using a cubed sphere grid. This type of dispersion analysis allows one to focus on group ($\partial\omega/\partial k$, where ω is the frequency and k is the wavenumber) and phase velocity ($\omega k/|k|^2$) for numerical discretizations. For RT_0, the numerical dispersion relation is very similar to the C grid finite difference numerical dispersion relation on quadrilaterals, with no turning points for the group velocity except at maximum wavenumbers. For RT_1, the numerical dispersion relation has two roots for each wavenumber, corresponding to the resolution of higher wavenumbers in the gridcell. When these are properly interpreted, the group velocity is mostly well-behaved except for a jump in the dispersion relation at Δx wavelengths where the group velocity goes to zero before and after the jump. Remarkably, the jump is repairable by modifying the coefficients in the mass matrix in such a way that the convergence rate is not eroded. It is not really the jump itself which is the problem, but the repair also makes the group velocity become non-zero through a L'Hôpital's rule type cancellation. This fix is independent of the value of f and H, so is useable in practice. In numerical experiments, Melvin *et al.* (2014) showed that this modification leads to propagation of a wave packet with Δx wavelength which otherwise stays in the same location, spuriously.

Eldred, Dubos and Kritsikis (2019) introduced an alternative approach to avoiding these dispersion relation spectral gaps, in which the nodal variables are the same as RT_0 and DG_0 on quadrilaterals, but a higher-order polynomial expansion is constructed by using nodal variables from surrounding cells. This can be seen as a form of spline, but does not increase the degree of continuity, just the polynomial degree. The effect on the numerical dispersion relation is that there is only one branch, so there cannot be jumps. The downside of this approach is that the stencil of the operators is extended to more cells, and the standard approach of finite element assembly becomes more complicated. Eldred and Le Roux (2018, 2019) examined the spectral gaps in RT_k elements for larger k, and showed that this spline approach also fixes the problem for higher k.

3.6. *Rossby waves*

Following the approach of Thuburn (2008), Cotter and Shipton (2012) also examined the Rossby wave propagation properties of compatible finite element spaces. Rossby waves occur in the situation where the Coriolis parameter f is spatially varying (as is the case on the sphere under the 'traditional approximation', where $f = 2\Omega \cdot n$, with Ω being the rotational velocity of the sphere, and n being the

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normal to the sphere surface). To perform the analysis, we consider solutions on an infinite plane, with $f = f_0 + \beta y$, where f_0 and β are constants. Then, if the Rossby number $\mathrm{Ro} = U/fL$ is small (where U is a typical velocity scale and L is a typical spatial scale), and also $\beta L/f_0 = O(\mathrm{Ro})$, then we neglect u_t and $\beta y u^\perp$ in the velocity equation. This gives the geostrophic balanced states $(u, h) = (u_g, \eta_g)$ satisfying

$$f_0 u_g^\perp = -g\nabla\eta_g, \tag{3.30}$$

so that $u_t = 0$, and $\eta_t = -H\nabla\cdot u = H\nabla\cdot(f_0\nabla^\perp\eta) = 0$, as we saw previously. This is the main reason why it is important for the discretization to represent these geostrophic balanced states. To obtain dynamics, we consider $O(\mathrm{Ro})$ corrections to (u, η), which we write as (u_{ag}, η_{ag}) (ageostrophic velocity and height). The equations at the next order in $O(\mathrm{Ro})$ then give

$$(u_g)_t + f_0 u_{ag}^\perp + \beta y u_g^\perp + g\nabla\eta_{ag} = 0, \quad (\eta_g)_t + H\nabla\cdot u_{ag} = 0. \tag{3.31}$$

Applying $-\nabla^\perp\cdot$ to the first equation and using the second gives

$$-\nabla^2\psi_t + \frac{f_0}{H}(\eta_g)_t - \beta u_g\cdot\hat{y} = 0, \tag{3.32}$$

where we used that $\nabla^\perp u_g = 0$, so $u_g = \nabla^\perp\psi$ (having already eliminating inertial oscillations which are fast), and $\hat{y}$ is the unit vector in the y-direction. Finally this becomes

$$\left(\frac{f_0^2}{gH} - \nabla^2\right)\psi_t - \beta\frac{\partial\psi}{\partial x} = 0, \tag{3.33}$$

which is the Rossby wave equation, which exhibits waves propagating westwards when $\beta > 0$ (i.e. in the Northern Hemisphere).

Now we examine what happens with compatible finite element discretizations in the low-Ro limit. At leading order in Rossby number, we obtain the geostrophic balance equation

$$\left\langle w, f u_g^\perp\right\rangle - g\langle\nabla\cdot w, \eta_g\rangle = 0 \quad \text{for all } w \in \mathbb{V}_h^1, \tag{3.34}$$

$$\langle\alpha, H\nabla\cdot u_g\rangle = 0 \quad \text{for all } \mathbb{V}_h^2. \tag{3.35}$$

We have already seen that this has solutions $u_g = \nabla^\perp\psi$, $h = P_2(f\psi)/h$ for $\psi \in \mathbb{V}_h^0$. At the next order we have

$$\langle w, (u_g)_t\rangle + \left\langle w, f_0 u_{ag}^\perp + \beta y u_g\right\rangle - \langle\nabla\cdot w, g\eta_{ag}\rangle = 0 \quad \text{for all } w \in \mathbb{V}_h^2, \tag{3.36}$$

$$\langle\alpha, (\eta_g)_t + H\nabla\cdot(u_g)\rangle = 0 \quad \text{for all } \alpha \in \mathbb{V}_h^1. \tag{3.37}$$

Choosing $w = \nabla^\perp\gamma$ with $\gamma \in \mathbb{V}_h^0$, and integrating by parts in (3.36) (permissible since $\gamma \in H^1$ and $u_{ag} \in H(\mathrm{div})$) gives

$$\langle\nabla\gamma, \nabla\psi\rangle - \langle\gamma, f\nabla\cdot u_{ag}\rangle - \langle\gamma, \beta\underbrace{u_g\cdot\hat{y}}_{=\partial\psi/\partial x}\rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}_h^0. \tag{3.38}$$

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Equation (3.37) implies that

$$f_0 P_2(\psi)/g + H\nabla \cdot u_g = 0 \quad \text{in } L^2. \tag{3.39}$$

Combining this with (3.38) then gives the discrete Rossby wave equation,

$$\langle \nabla\gamma, \nabla\psi_t \rangle + \left\langle \gamma, \frac{f_0^2}{gH} P_2\psi \right\rangle - \left\langle \gamma, \beta \frac{\partial \psi}{\partial x} \right\rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}_h^0. \tag{3.40}$$

Without the P_2 projection operator, this would just be a regular H^1 finite element approximation of the Rossby wave equation. With it, there is the possibility of some projection errors altering the numerical dispersion relation, especially in the case of BDM elements where $\dim(\mathbb{V}_h^0) > \dim(\mathbb{V}_h^2)$. However, this will only occur for high-wavenumber waves, where the dynamics is already dominated by the Laplacian term, and the Rossby waves will have very slow phase and group velocities in either case. Hence we do not believe that this causes a problem for discrete Rossby wave propagation. A similar argument was made in Thuburn (2008) when considering C grid discretizations on hexagons.

Rostand and Le Roux (2008) examined the wave propagation properties of the RT_0–DG_0 and BDM_1–DG_0 compatible finite element discretizations (and RT_0–CG_1 and BDM_1–CG_1 discretizations that are not compatible) using discrete dispersion relations computed through Fourier analysis. These dispersion relations revealed the steady geostrophic modes for constant f, and two branches of the dispersion relation for BDM_1–DG_0, a primary one attached to the origin (zero frequency for zero wavenumber) and a secondary one which they described as spurious. It is possible that this second branch can be interpreted as corresponding to higher wavenumbers resolved in the cell, just as for RT_1 on quadrilaterals as explored by Staniforth *et al.* (2013), but doing these calculations is difficult on triangles and more work is needed to clarify this. In their dispersion analysis, Rostand and Le Roux (2008) identified 'CD modes' in the BDM_1–DG_0 discretization, which are modes in the intersection of the Coriolis operator and the divergence operator. These precisely correspond to the modes in the kernel of the P_2 operator appearing in (3.40). In experiments with the linear rotating shallow water equations with balanced initial data and $f = f_0 + \beta y$, designed to examine Rossby wave propagation, they observed accurate solutions on structured grids but very noisy solutions on unstructured grids. The noise was attributed to interactions with the CD modes. However, when we have repeated these experiments using modern automated finite element systems such as FEniCS and Firedrake, we have not observed this noisy behaviour with BDM_1 on unstructured grids. It seems likely that Rostand and Le Roux (2008) had bugs in their implementation related to the identification of the two nodal variables between two cells across each edge (since no such problem arose with RT_0, which only has one nodal variable per edge). This is understandable, because the problem of how to systematically assemble BDM_1 and higher-order $H(\mathrm{div})$ spaces on triangles was not solved until Rognes *et al.* (2010); these things are very difficult to implement by hand. These results

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may have discouraged the adoption of the BDM family for atmosphere and ocean modelling, but it seems like a good option for lowest-order spaces to avoid the issues with spurious inertia–gravity wave propagation with RT_0.

3.7. *Consistent linear tidal response*

Cotter and Kirby (2016) considered solutions of the linearized barotropic tide equations, which take the form

$$u_t + fu^\perp + g\nabla(D + b) = -cu + F, \quad D_t + H\nabla \cdot u = 0. \tag{3.41}$$

These are the linear rotating shallow water equations with additional topography b, spatiotemporal lunar forcing F and linear friction coefficient c. They used the Helmholtz equation to obtain an exponentially damping lower and upper bound on the energy in the absence of forcing. In the presence of time-dependent forcing (quasiperiodic forcing is appropriate for tidal models), they proved that the solution converges at exponential rate to a time-dependent solution as $t \to \infty$, independent of the initial condition. This is the solution that is of interest when predicting tides. When compatible finite element methods are used to discretize the tide equations, they proved that the continuous-time discrete-space solution also converges exponentially to a time-dependent numerical solution, independent of the initial condition. Finally they showed that this discrete attracting solution converges to the unapproximated attracting solution as the mesh is refined. Cotter, Graber and Kirby (2018) extended this analysis to a nonlinear model with cu replaced by $c|u|u$, which is the more realistic damping model that is actually used by oceanographers. This nonlinear case is surprisingly subtle but they were able to prove long-time stability of the system and obtain rates of damping in the unforced case. These were used to prove error estimates for the discrete solution obtained using compatible finite element methods. Kirby and Kernell (2021) used the compatible finite element framework to design a preconditioner for the implicit solver for the tidal equations, proving that the convergence rates are independent of mesh resolution. Cotter, Kirby and Morris (2022) extended this approach to the multiple layer version of this model.

3.8. *Hydrostatic balance*

Finally in this section, we discuss the discrete hydrostatic balance properties of compatible finite element methods. Later, we shall introduce three-dimensional geophysical fluid dynamics models with gravity and pressure gradient terms, so that the velocity equation takes the form

$$\frac{\partial u}{\partial t} + \cdots + \underbrace{\nabla p}_{\text{pressure gradient}} = \underbrace{b\hat{k}}_{\text{gravity}}, \tag{3.42}$$

in the case of the Boussinesq equations (typically used in ocean modelling), where p is the pressure, b is the buoyancy and $\hat{k}$ is the unit normal vector in the 'up'

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direction. In the case of the compressible Euler equations (typically used in atmosphere modelling), we have

$$\frac{\partial u}{\partial t} + \cdots + c_p \underbrace{\theta \nabla \Pi}_{\text{pressure gradient}} = \underbrace{-g\hat{k}}_{\text{gravity term}}, \tag{3.43}$$

where θ is the potential temperature, Π is the Exner pressure and g is the acceleration due to gravity. In both cases we are concerned with states of hydrostatic balance, which is when the vertical component of the pressure gradient term balances the gravity term. Either we are considering hydrostatic models, where this balance is enforced exactly in the model, or we are considering non-hydrostatic models where it is important that these hydrostatic states can be accurately represented. In the compatible finite element case, to study the vertical part of the velocity equation, we restrict the test function in the velocity equation to $\mathbb{W}_h^{2,V}$ (assuming a tensor product discrete de Rham complex), the vertical part of the space $\mathbb{W}_h^2$ containing the discretized velocity u.

In the case of the Boussinesq equations, the discrete hydrostatic balance is written (after integration by parts) as

$$-\langle \nabla \cdot w, p \rangle = \langle w \cdot \hat{k}, b \rangle \quad \text{for all } w \in \mathring{\mathbb{W}}_h^{2,V}, \tag{3.44}$$

for pressure $p \in \mathbb{W}_h^3$ and buoyancy $b \in \mathbb{W}_h^\theta$, where $\mathring{\mathbb{W}}_h^{2,V}$ is the subspace of the vertical space $\mathbb{W}_h^{2,V}$ requiring the boundary condition $u \cdot n = 0$ at the top and the bottom. Despite appearances, this is actually only defining the vertical part of the pressure gradient term, since $w \in \mathring{\mathbb{W}}_h^{2,V}$ always points in the vertical direction.

Given p, there is a unique b that satisfies this hydrostatic balance. To see this, we note that if the layers of the mesh are flat, then $w \cdot k \in \mathbb{W}_h^\theta$ for all $w \in \mathbb{W}_h^{2,V}$. If the layers are not flat, i.e. for terrain-following coordinates, then there exists $0 \leq \kappa \leq \infty$ such that $\kappa w \cdot k \in \mathbb{W}_h^\theta$ for all $w \in \mathbb{W}_h^{2,V}$. After replacing $w \cdot k = \kappa^{-1}\gamma$ for $\gamma \in \mathbb{W}_h^\theta$, we recognize the right-hand side of (3.44) as a non-degenerate weighted L^2 inner product, hence b is unique.

To discuss the nature of the uniqueness of p, we consider an alternative boundary condition with $u \cdot n = 0$ on the bottom, and $p = p_0$ on the top (for some chosen p_0 which may depend on the horizontal coordinate). The equation after integration by parts and use of the top boundary condition gives

$$-\langle \nabla \cdot w, p \rangle + \langle\langle w \cdot n, p_0 \rangle\rangle = \langle w \cdot \hat{k}, b \rangle \quad \text{for all } w \in \mathring{\mathbb{W}}_h^{2,V}, \tag{3.45}$$

where $\mathring{\mathbb{W}}_h^{2,V}$ is now the subspace with vanishing normal component on the bottom only. To analyse this problem, Natale *et al.* (2016) introduced the following formulation, defining $(v, p) \in \mathbb{W}_h^{2,V} \times \mathbb{W}_h^3$ such that

$$\langle w, v \rangle - \langle \nabla \cdot w, p \rangle = \langle w \cdot \hat{k}, b \rangle - \langle\langle w \cdot n, p_0 \rangle\rangle \quad \text{for all } w \in \mathring{\mathbb{W}}_h^{2,V}, \tag{3.46}$$

$$\langle \phi, \nabla \cdot v \rangle = 0 \quad \text{for all } \phi \in \mathbb{W}_h^3, \tag{3.47}$$

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which we recognize as a mixed problem defined on $\mathbb{W}_h^{2,V} \times \mathbb{W}_h^3$. Using the same arguments as earlier, at the solution we have $\nabla \cdot v = 0$ in L^2. Since $v \cdot n = 0$ on the bottom surface, and v points in the vertical direction, we conclude that $v = 0$, and therefore p solves (3.45). Natale *et al.* (2016) showed that this type of vertical mixed problem has a unique solution (v, p). Hence there is a one-to-one correspondence between p and b, as required. If there are boundary conditions $u \cdot n = 0$ on both top and bottom surfaces, p is only determined up to the value p_0 restricted to the upper surface, also as required.

In the case of the compressible Euler equations, taking boundary conditions $u \cdot n = 0$ on the bottom surface and $\Pi = \Pi_0$ on the top surface, the discrete hydrostatic balance is written (after integrating by parts) as

$$-\langle \nabla \cdot (\theta w), \Pi \rangle = \langle w \cdot \hat{k}, g \rangle - \langle\!\langle w \cdot n, \Pi_0 \rangle\!\rangle \quad \text{for all } w \in \mathring{\mathbb{W}}_h^{2,V}, \tag{3.48}$$

for $\Pi \in \mathbb{W}_h^3$ and $\theta \in \mathbb{W}_h^\theta$. Using an extension of the techniques described for the Boussinesq equation, Natale *et al.* (2016) proved similar results. This motivates the use of $\mathbb{W}_h^\theta$ for temperature variables like b or θ. Melvin, Benacchio, Thuburn and Cotter (2018) showed through linear dispersion analysis applied to the compressible Boussinesq equations that this choice does indeed lead to an absence of spurious hydrostatic modes that would appear if $\theta \in \mathbb{W}_h^3$ or $\mathbb{W}_h^0$.

4. Transport and stabilization

Hopefully it is clear from Section 3 that it might be interesting to consider designing a numerical atmosphere or ocean model using compatible finite element methods. One very important aspect of these models is the choice of transport schemes, i.e. the discretization of the advection operators. Since different fields are restricted to different spaces from the discrete de Rham complex (or $\mathbb{W}_h^\theta$) with different continuity constraints, we need to consider a diverse range of transport schemes, some of which we briefly survey in this section.

4.1. Transport of H^1 fields

For scalar fields in $\mathbb{W}_0$ or $\mathbb{V}_0$ (we will call it V here), we consider the discretization of the advection equation

$$\frac{\partial q}{\partial t} + u \cdot \nabla q = 0, \tag{4.1}$$

for some specified $u \in \mathbb{W}_h^2$ or $\mathbb{V}_h^1$, where we assume that $u \cdot n = 0$ on exterior boundaries. Since V is a continuous finite element space, we simply take the L^2 inner product with a test function and integrate by parts to obtain the standard continuous finite element approximation, seeking $q \in V$ such that

$$\left\langle \phi, \frac{\partial q}{\partial t} \right\rangle - \langle \nabla \cdot (u\phi), q \rangle = 0 \quad \text{for all } \phi \in V. \tag{4.2}$$

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As is well known, this discretization tends to produce spurious oscillations at regions of rapid changes in q. One way to suppress these oscillations is to use the streamline upwind Petrov–Galerkin (SUPG) method (Brooks and Hughes 1982, Tezduyar, Glowinski and Liou 1988, Tezduyar 1989). In this approach, the test function ϕ is replaced by $\phi + \tau u \cdot \nabla\phi$, which biases it in the upwind direction; τ is some chosen stabilization parameter which depends on the mesh, u and other parameters. This leads to

$$\left\langle \phi + \tau u \cdot \nabla\phi, \frac{\partial q}{\partial t} \right\rangle - \langle \nabla \cdot (u\phi), q \rangle + \langle \tau u \cdot \nabla\phi, u \cdot \nabla q \rangle = 0 \quad \text{for all } \phi \in V. \tag{4.3}$$

The final term performs diffusion along streamlines of u, which tends to reduce spurious oscillations. By applying this modification in the $\partial q/\partial t$ term as well as the $u \cdot \nabla q$ term, we obtain a consistent approximation (i.e. substituting a smooth exact solution of the unapproximated equation produces zero).

Another possibility is the edge stabilization approach proposed for advection equations and analysed (when combined with diffusion) in Burman and Hansbo (2004), resulting in the formulation

$$\left\langle \phi, \frac{\partial q}{\partial t} \right\rangle - \langle \nabla \cdot (u\phi), q \rangle + \langle\!\langle \gamma h^2 [\![\nabla\phi]\!], [\![\nabla q]\!] \rangle\!\rangle_\Gamma = 0 \quad \text{for all } \phi \in V, \tag{4.4}$$

where

$$\langle\!\langle u, v \rangle\!\rangle_\Gamma = \int_\Gamma u \cdot v \, \mathrm{d}S, \tag{4.5}$$

Γ is the union of all interior facets f in the mesh (i.e. facets joining two cells), $[\![v]\!] = v^+ n^+ + v^- n^-$ for vector fields v, each facet f has been arbitrarily assigned $+$ and $-$ labels to its two sides, $a^\pm$ indicates the restriction of the discontinuous function a to the $\pm$ side of the facet, respectively, h is a mesh edge length parameter, and γ is a (possibly u- or q-dependent) stabilization parameter. This term has a diffusive effect across interior facets, penalizing jumps in q, without sacrificing consistency as $h \to 0$.

4.2. *Transport of L^2 fields*

The spaces $\mathbb{W}_h^3$ and $\mathbb{V}_h^2$ have no continuity constraints, which allows for upwind stabilization via a discontinuous Galerkin formulation. Here we consider the continuity equation

$$D_t + \nabla \cdot (uD) = 0, \tag{4.6}$$

where u is as above. We introduce the discretization by multiplying by a test function and integrating over a single mesh cell e,

$$\int_e \phi D_t - \nabla\phi \cdot uD \, \mathrm{d}x + \int_{\partial e} \tilde{D} u \cdot n \phi \, \mathrm{d}S = 0 \quad \text{for all } \phi \in V(e), \tag{4.7}$$

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where ∂e is the boundary of e with outward-pointing normal n, V is the chosen discontinuous space, and $\tilde{D}$ is the upwind value of D, which must be defined in terms of the values of D on the inside and the outside of e. When $u \cdot n > 0$, then $\tilde{D}$ is equal to D from inside e, otherwise the outside value is used. If we sum over all the cells e in the mesh, we obtain

$$\langle \phi, D_t \rangle - \langle \nabla_h \phi, uD \rangle + \langle\!\langle [\![\phi u]\!], \tilde{D} \rangle\!\rangle_\Gamma = 0 \quad \text{for all } \phi \in V(\Omega), \tag{4.8}$$

where ∇_h indicates the cellwise 'broken' gradient,

$$\nabla_h|_e D = \nabla|_e D, \tag{4.9}$$

for each cell e in the mesh. An analysis of how this choice of upwind $\tilde{D}$ introduces stabilization is provided in Brezzi, Marini and Süli (2004). This method is locally conservative.

4.3. *Transport of H(div) fields*

In consideration of the $(u \cdot \nabla)u$ term in the velocity equation of geophysical models, and discretizations for vector advection equations of the form

$$\frac{\partial v}{\partial t} + (u \cdot \nabla)v = 0, \tag{4.10}$$

for a vector field v in H(div) spaces $\mathbb{W}_h^{2,V}$ or $\mathbb{V}_h^1$, u is again as above. When the equation is solved on surface of the sphere, v is constrained to be tangential to the sphere (or the mesh approximating the sphere in the discrete case). Then the equation becomes

$$\frac{\partial v}{\partial t} + \mathbb{P}_S((u \cdot \nabla)v) = 0, \tag{4.11}$$

where $\mathbb{P}_S$ is the Euclidean projection into the tangent plane to the sphere.

Functions in H(div) spaces are only partially continuous (in the normal component across facets), so we need to start by considering an upwind formulation on a single cell again,

$$\int_e w \cdot v_t - \nabla \cdot (u \otimes w) \cdot v \, \mathrm{d}x + \int_{\partial e} n \cdot uw \cdot \tilde{v} \, \mathrm{d}S = 0 \quad \text{for all } w \in V(e), \tag{4.12}$$

where $(a \otimes b)_{ij} = a_i b_j$ for vectors a and b, $\tilde{v}$ is the upwind value of v, $A : B = \sum_{ij} A_{ij} B_{ij}$ for two matrices A and B, and V is the chosen H(div) space. Summing up over all of the cells in the mesh gives

$$\int_\Omega w \cdot v_t - \nabla_h \cdot (u \otimes w) \cdot v \, \mathrm{d}x + \int_{\partial\Gamma} [\![u \otimes w]\!] \cdot \tilde{v} \, \mathrm{d}S = 0 \quad \text{for all } w \in V(\Omega), \tag{4.13}$$

where $[\![u \otimes w]\!] = (n^+ \cdot u^+)w^+ + (n^- \cdot u^-)w^-$. Since $v \in V$ has continuous normal components, $\tilde{v}$ only differs from v in the tangential component. Hence the upwind stabilization may be insufficient to adequately suppress oscillations, depending on

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the shape of the mesh cells and the direction of the velocity. On meshes approximating the sphere (and other manifolds), these formulae require modification when $n^+ \neq -n^-$ on an edge. The modification rotates $\tilde{u}$ into the tangent plane of the cell e, as described in Bernard *et al.* (2009). The projection of the advection equation into the tangent to the sphere is naturally dealt with in (4.13), because $w \in \mathbb{V}_h^2$ is always tangential to the surface mesh.

The vorticity form is an alternative form of the vector advection equation, given by

$$\frac{\partial v}{\partial t} + (\nabla \times v) \times u + \frac{1}{2}\nabla(u \cdot v) + \frac{1}{2}\left((\nabla v)^\top u - (\nabla u)^\top v\right) = 0, \tag{4.14}$$

in three dimensions, where $(\nabla v)^\top_{ij} = \partial u_j / \partial x_i$. In two dimensions this is written as

$$\frac{\partial v}{\partial t} + (\nabla^\perp \cdot v) \cdot u^\perp + \frac{1}{2}\nabla(u \cdot v) + \frac{1}{2}\left((\nabla v)^\top u - (\nabla u)^\top v\right) = 0, \tag{4.15}$$

where

$$w^\perp = (-w_2, w_1), \quad \omega = \nabla^\perp \cdot w := -\frac{\partial w_2}{\partial x_1} + \frac{\partial w_1}{\partial x_2} \tag{4.16}$$

for a vector field w in planar geometry. On the sphere, with outward-pointing normal $\hat{k} = x/|x|$ (and x is the three-dimensional coordinate with origin at the centre of the sphere), we have $w^\perp = \hat{k} \times w$ and $\nabla^\perp \cdot w = \hat{k} \cdot \nabla \times w$, where ∇ is now the projection of the gradient into the tangent to the mesh surface; see Rognes, Ham, Cotter and McRae (2013) for implementation details.

When $v = u$, we have the 'vector-invariant' form

$$\frac{\partial u}{\partial t} + \underbrace{(\nabla \times u) \times u}_{\text{or } (\nabla^\perp \cdot u) u^\perp} + \frac{1}{2}\nabla |u|^2 = 0, \tag{4.17}$$

which is particularly useful on the surface of the sphere because it avoids the need to rotate upwinded vectors. To see this, we multiply by a test function $w \in V$ and integrate over one cell, integrating by parts to get

$$\int_e w \cdot \frac{\partial u}{\partial t} - \nabla^\perp(w \cdot u^\perp) \cdot u - \nabla \cdot w \frac{1}{2}|u|^2 \,\mathrm{d}x + \int_{\partial e} w \cdot u^\perp n^\perp \cdot \tilde{u} \,\mathrm{d}S = 0 \quad \text{for all } w \in V. \tag{4.18}$$

Here no rotation is required because the tangent to the edge between cells agrees on both sides: it is just the facet normal (the normal to the cell edge that is tangential to the cell surface) that can change on manifold meshes. Summing over all of the cells in the mesh gives

$$\int_\Omega w \cdot \frac{\partial u}{\partial t} - \nabla^\perp(w \cdot u^\perp) \cdot u - \nabla \cdot w \frac{1}{2}|u|^2 \,\mathrm{d}x - \int_\Gamma [\![w \cdot u^\perp]\!] \cdot \tilde{u}^\perp \,\mathrm{d}S = 0, \tag{4.19}$$

where for scalars ϕ, $[\![\phi]\!] = \phi^+ n^+ + \phi^- n^-$. This upwinded vector-invariant form for $H(\mathrm{div})$ spaces first appeared in Natale and Cotter (2018) for the incompressible

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Euler equations, and was used for the rotating shallow water equations on the sphere in Gibson *et al.* (2019).

The polynomial spaces for lowest-order RT elements do not span all linear vector fields. This means that if we use the above scheme then it will only be first-order accurate. Bendall and Wimmer (2023) looked at using an auxiliary field $q \in \mathbb{V}_h^0$ with $q = -\delta_0 v$, that is, q approximates $\nabla^\perp \cdot v$ if the solution domain Ω has no boundary. Then we can use this in an approximation of (4.15):

$$\left\langle w, \frac{\partial v}{\partial t} \right\rangle + \langle w, q u^\perp \rangle - \frac{1}{2}\langle \nabla \cdot w, u \cdot v \rangle + G'(v; w) \quad \text{for all } w \in \mathbb{V}_h^1. \tag{4.20}$$

This was inspired by the energy–enstrophy conserving schemes that we discuss in Section 7. Here, G' represents the discretization of the last two terms on the left-hand side of (4.15), which we do not go into here (standard upwind discontinuous Galerkin approaches were used, similar to those above). To obtain the dynamics for q, we can select $w = -\nabla^\perp \gamma$ for $\gamma \in \mathbb{V}_h^0$, and substitute into (4.20) to obtain

$$\left\langle \gamma, \frac{\partial q}{\partial t} \right\rangle - \langle \nabla \gamma, q u \rangle - G'(v; \nabla^\perp \gamma) \quad \text{for all } \gamma \in \mathbb{V}_h^0. \tag{4.21}$$

We recognize the first two terms as the standard continuous finite element approximation of $\partial q/\partial t + u \cdot \nabla q$. As we discussed above, some method of stabilization is usually needed to suppress oscillations in this approximation. Modifying the test function according to the SUPG approach is ungainly here, because of the surface terms in G'. Instead, Bendall and Wimmer (2023) used a residual-based approach, writing

$$\left\langle \gamma, \frac{\partial q}{\partial t} \right\rangle - \langle \nabla \gamma, q^* u \rangle - G'(v; \nabla^\perp \gamma) \quad \text{for all } \gamma \in \mathbb{V}_h^0, \tag{4.22}$$

where

$$q^* = q - \tau \left(\frac{\partial q}{\partial t} + \nabla \cdot (uq) + \frac{1}{2} \nabla_h^\perp \left((\nabla_h v)^\top u - (\nabla_h u)^\top v \right) \right), \tag{4.23}$$

where τ is a stabilization parameter. We note that this change preserves the consistency of the discretization since the quantity in the brackets is just the curl $(\nabla^\perp \cdot)$ of (4.15). Then the equation for v becomes

$$\left\langle w, \frac{\partial v}{\partial t} \right\rangle + \langle w, q^* u^\perp \rangle - \frac{1}{2}\langle \nabla \cdot w, u \cdot v \rangle + G'(v; w) \quad \text{for all } w \in \mathbb{V}_h^1. \tag{4.24}$$

Bendall and Wimmer (2023) showed in numerical experiments (including a nonlinear rotating shallow water equation test case on the sphere) that this discretization produces second-order accurate solutions using lowest-order RT quadrilateral elements on a cubed sphere grid, whilst (4.19) only produces first-order accurate solutions. A predecessor of this scheme was considered in Kent, Melvin and Wimmer (2023), but without the consistent definition of q and u.

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Transport schemes for $\mathbb{W}_h^1$ are discussed in Wimmer and Tang (2022) in the context of magnetohydrodynamics, using similar ideas to those discussed in this section for $\mathbb{W}_h^2$.

4.4. *Temperature space transport schemes*

The temperature space $\mathbb{W}^\theta$ produces similar challenges, since it is continuous in the vertical and discontinuous in the horizontal. Yamazaki *et al.* (2017) combined an upwind discontinuous Galerkin discretization in the horizontal with an SUPG discretization in the vertical, with the modification of test functions $\gamma \mapsto \gamma + \tau\hat{k} \cdot u\, \partial\tau/\partial z$, producing a second-order scheme when the RT_1 discrete de Rham complex is used, so that temperature is continuous quadratic in the vertical and discontinuous linear in the horizontal.

In staggered grid weather models, it is standard practice to collocate thermodynamic tracers such as moisture, etc., with temperature. This makes it easier to localize thermodynamic processes that alter, and depend on, the temperature (see e.g. Bush *et al.* 2020). Hence we need to use $\mathbb{W}_h^\theta$ transport schemes for those tracers as well. For many of these tracers (moisture, chemical species, etc.) it is important to avoid numerical over- and undershoots leading to negative humidity, for example. Hence it is important to be able to incorporate limiters into $\mathbb{W}_h^\theta$ transport schemes. Cotter and Kuzmin (2016) proposed such a scheme for the vertically quadratic, horizontally linear $\mathbb{W}_h^\theta$ also considered by Yamazaki *et al.* (2017). In that scheme, at the beginning of the time-step, the vertical continuity conditions are relaxed, and an upwind discontinuous Galerkin transport scheme is applied over one time-step in $\hat{\mathbb{W}}_h^\theta$, the corresponding discontinuous space. A slope limiter, such as the one in Kuzmin (2013), can then be used to avoid under- and overshoots in this step. Then an element-based flux-corrected remapping is used to transform θ back to the vertically continuous space $\mathbb{W}_h^\theta$. The flux correction switches between a high-order and low-order mapping in order to maximize the use of the high-order solution unless under- or overshoots would otherwise occur.

4.5. *Recovered space schemes*

The lowest-order RT de Rham complex on hexahedra is attractive because it allows storage of field values at the same grid locations as for the C grid finite difference approximation. This is why this de Rham complex is being used for the Met Office 'GungHo' dynamical core (Melvin *et al.* 2019). However, as we have already mentioned above, standard upwind finite element schemes on these spaces are only first-order accurate, because only $\mathbb{W}_h^0$ has element shape functions that span the complete linear polynomial space; $\mathbb{W}_h^i$, $i = 1, 2, 3$, and $\mathbb{W}_h^\theta$ do not. Bendall, Cotter and Shipton (2019) chose to address this by using recovery operators to construct higher-order approximations of the solution based on averaging cell values around vertices. If the original low-order solution is obtained by interpolating a smooth

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function, this recovery step produces a higher-order continuous finite element solution (Georgoulis and Pryer 2018). Following Cotter and Kuzmin (2016), they then relaxed the continuity of the higher-order recovered solution and applied a discontinuous Galerkin transport scheme step before remapping back to the original low-order finite element spaces. This was demonstrated in numerical experiments to produce second-order convergence of solutions. Bendall and Wimmer (2023) introduced modifications to extend this approach to the sphere.

This recovery process also allows the introduction of limiters to prevent over- and undershoots. This was done in Bendall *et al.* (2020), applied to compressible Euler solutions with moisture, where limiters are critical for stability. This produced the first atmospheric simulations using compatible finite elements with moist physics. Bendall, Wood, Thuburn and Cotter (2022) then showed how to achieve this framework whilst conserving mass and total moisture.

5. Example discretizations and iterative solution strategies

In this section we survey some compatible finite element discretizations of geophysical fluid dynamics models, concentrating on approaches that can be considered as evolutions of existing approaches using more 'traditional' discretizations. More advanced structure preserving discretizations are discussed in Sections 6–9.

5.1. Rotating shallow water equations on the sphere

We start with the rotating shallow water equations on the sphere, written as

$$\frac{\partial u}{\partial t} + \mathbb{P}_S((u\cdot\nabla)u) + fu^\perp + g\nabla(D+b) = 0, \tag{5.1}$$

$$\frac{\partial D}{\partial t} + \nabla\cdot(Du) = 0, \tag{5.2}$$

where u is the horizontal velocity tangential to the sphere, D is the depth of the fluid layer and b is the height of the bottom surface.

Gibson *et al.* (2019) introduced a spatial discretization built around the vector-invariant formulation (4.19) for velocity advection u, and the discontinuous Galerkin formulation (4.8) for depth D. This leads to a spatial discretization seeking $(u, D) \in \mathbb{V}_h^1 \times \mathbb{V}_h^2$ such that

$$\left\langle w, \frac{\partial u}{\partial t}\right\rangle - \left\langle \nabla_h^\perp(w\cdot u^\perp), u\right\rangle + \langle\!\langle [\![w\cdot u^\perp]\!], \tilde{u}^\perp \rangle\!\rangle_\Gamma$$
$$- \nabla\cdot w\left(\frac{1}{2}|u|^2 + g(D+b)\right) \mathrm{d}x = 0 \quad \text{for all } w \in \mathbb{V}_h^1, \tag{5.3}$$

$$\langle \phi, D_t\rangle - \langle \nabla_h\phi, uD\rangle + \langle\!\langle [\![\phi u]\!], \tilde{D}\rangle\!\rangle_\Gamma = 0 \quad \text{for all } \phi \in \mathbb{V}_h^2. \tag{5.4}$$

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They used a semi-implicit time-stepping scheme, which is best described as some form of iteration towards the fully implicit time-stepping scheme

$$\begin{aligned}\left\langle w, u^{n+1}-u^n\right\rangle - \Delta t\left\langle \nabla_h^\perp(w\cdot\bar{u}^\perp), \left(u^{n+1/2}\right)^\perp\right\rangle \\ + \Delta t\left\langle\!\!\left\langle [\![w\cdot\bar{u}^\perp]\!], \left(\tilde{u}^{n+1/2}\right)^\perp\right\rangle\!\!\right\rangle_\Gamma \\ - \Delta t\nabla\cdot w\left(\frac{1}{2}|\bar{u}|^2 + g(\bar{D}+b)\right)\mathrm{d}x = 0 \quad \text{for all } w\in\mathbb{V}_h^1, \qquad (5.5)\end{aligned}$$

$$\langle\phi, D_t\rangle - \Delta t\langle\nabla_h\phi, \bar{u}D\rangle + \Delta t\left\langle\!\!\left\langle [\![\phi\bar{u}]\!], \tilde{D}\right\rangle\!\!\right\rangle_\Gamma = 0 \quad \text{for all } \phi\in\mathbb{V}_h^2, \qquad (5.6)$$

where $u^{n+1/2} = \bar{u} = (u^{n+1}+u^n)/2$. This mixture of two symbols for the same thing is introduced to describe an iteration based around this implicit discretization. We write $v^0 = u^n, v^1, v^2, \ldots$ and $D^0 = D^n, D^1, D^2, \ldots$ as a sequence of iterative approximations to u^{n+1} and u^n, respectively. For each iteration k, we write $\bar{u} = (u^n + v^k)/2$, $\bar{D} = (D^n + D^k)/2$, solving (5.5)–(5.6) for u^{n+1} and D^{n+1} using those values of $\bar{u}$ and $\bar{D}$. Then we use the linearization about the state of rest to compute iterative corrections $(\Delta u, \Delta D)$, according to

$$\begin{aligned}\langle w, \Delta u\rangle + \frac{\Delta t}{2}\langle w, f\Delta u^\perp\rangle \\ - \frac{\Delta t}{2}\langle\nabla\cdot w, g\Delta D\rangle = -R_u[w] := -\left\langle w, u^{n+1}-u^n\right\rangle \quad \text{for all } w\in\mathbb{V}_h^1, \qquad (5.7)\end{aligned}$$

$$\left\langle \phi, \Delta D + \frac{H\Delta t}{2}\nabla\cdot\Delta u\right\rangle = -R_D[\phi] := -\left\langle\phi, D^{n+1}-D^n\right\rangle \quad \text{for all } \phi\in\mathbb{V}_h^2. \qquad (5.8)$$

We will discuss the solution of this linear system later. The time integration scheme applies a fixed number of iterations of this type (typically $2 \le k_{\max} \le 4$). We then take $(u^{n+1}, D^{n+1}) = (v^{k_{\max}}, D^{k_{\max}})$ before moving to the next time-step. It is not intended to converge to the solution of the implicit midpoint rule but just to produce a second-order semi-implicit scheme that is stable conditional on the advective Courant number $|u|\Delta t/\Delta x$, but unconditionally in the wave Courant number $\sqrt{gH}\Delta t/\Delta x$. A probably more stable approach is to use the form (4.15) for the velocity equation, substituting $\bar{u}$ for u and u for v. This was done using quadrilateral RT_0 elements in Bendall and Wimmer (2023). Another approach is to replace the implicit midpoint rule update for u^{n+1} and D^{n+1} given $\bar{u}$, instead using an explicit transport step (or several substeps). This can facilitate more sophisticated transport schemes with limiters that are hard to implement in implicit schemes. This was also done using quadrilateral RT_0 elements in Bendall and Wimmer (2023).

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5.2. *Rotating incompressible Boussinesq equations*

For ocean models, the most common setting is the incompressible Boussinesq equations,

$$\frac{\partial u}{\partial t} + (u \cdot \nabla)u + 2\Omega \times u + \nabla p - b\hat{k} = 0, \tag{5.9}$$

$$\frac{\partial b}{\partial t} + (u \cdot \nabla)b = 0, \tag{5.10}$$

$$\nabla \cdot u = 0, \tag{5.11}$$

where Ω is the Earth's rotation rate, p is the pressure and b is the buoyancy. Here we limit discussion to the rigid lid approximation with boundary conditions $u \cdot n = 0$ on all boundaries. In full ocean models there are generally two thermodynamic tracers, the potential temperature θ and the salinity S, which are both transported by advection equations as b is above, and b is then a specified function of θ and S via an equation of state. However, here we keep things to the simple formulation above. Further, many models make the hydrostatic approximation, but we do not discuss that here. Finally, these equations are extended in operational models to include mixing parametrizations and representations of other physical processes; we do not discuss those either.

Yamazaki *et al.* (2017) introduced a hybrid approach for velocity advection in the vertical slice setting (the velocity is three-dimensional but all fields are independent of y, so the equations can be solved on a two-dimensional mesh in the $x-z$ plane), with (4.19) as the transport scheme for the $x-z$ components of velocity, and a standard upwind discontinuous Galerkin scheme for the y component. For buoyancy b (represented in $\mathbb{W}^\theta$), the hybrid scheme with upwind discontinuous Galerkin in the horizontal and SUPG in the vertical was used. This spatial discretization was combined with a time-stepping scheme similar to the one above, resulting in a linear system of the form

$$\begin{aligned}
&\langle w, \Delta u\rangle + \frac{\Delta t}{2}\langle w, 2\Omega \times \Delta u\rangle \\
&- \frac{\Delta t}{2}\langle \nabla \cdot w, \Delta p\rangle - \langle w, b\hat{k}\rangle = -R_u[w] \quad \text{for all } w \in \mathbb{W}_h^2,
\end{aligned} \tag{5.12}$$

$$\langle \gamma, \Delta b\rangle + \frac{\Delta t}{2}\langle \gamma, \Delta u \cdot \hat{k} B_z\rangle = -R_b[\gamma] \quad \text{for all } \gamma \in \mathbb{W}_h^\theta, \tag{5.13}$$

$$\langle \phi, \nabla \cdot \Delta u\rangle = 0 \quad \text{for all } \phi \in \mathbb{W}_h^3, \tag{5.14}$$

where B_z is the vertical derivative of a reference buoyancy profile, to compute the iterative linear corrections to u^{n+1}, p^{n+1} (actually an approximation to pressure at time level $t^{n+1/2}$) and b^{n+1}, analogously to (5.7)–(5.8).

Equations (5.12)–(5.14) were solved by eliminating Δb. This is possible without introducing errors on an extruded mesh with flat layers when B_z is constant, since $\Delta b\hat{k} \in \mathbb{W}_h^{2,V}$. When that is not the case, the errors from the approximate elimination

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can be removed by using the elimination as a preconditioner for a Krylov method on (5.12)–(5.14). At the time, the equations were modified by setting Ω to zero on the left-hand side (which prevented the iterative solver from being robust to large values of Ω), and using GMRES applied to the coupled system

$$\left\langle w, \Delta u + \frac{\Delta t^2}{4}\hat{k}\hat{k}\Delta u B_z \right\rangle + \frac{\Delta t}{2}\langle w, 2\Omega \times \Delta u\rangle - \frac{\Delta t}{2}\langle \nabla \cdot w, \Delta p\rangle - \langle w, b\hat{k}\rangle = -\tilde{R}_u[w] \quad \text{for all } w \in \mathbb{W}_h^2, \tag{5.15}$$

$$\nabla \cdot \Delta u = 0. \tag{5.16}$$

This was preconditioned by an $H(\mathrm{div})$ block preconditioner, which we do not describe here. However, it is much better to precondition (5.15)–(5.16) using a hybridized solver, which we describe later in this section.

Yamazaki *et al.* (2017) showed that this suite of discretization and solver choices produces a scheme that can resolve fronts in the Eady vertical slice frontogenesis problem to a similar degree as C grid finite difference methods used previously. After this paper was published, the authors experimented with replacing the hybrid advection scheme for velocity with a full vector-invariant form in all three components of velocity. In this case, oscillations in the velocity field quickly emerge when the front sharpens. These oscillations do not appear when (4.13) is used instead. It is possible that this is related to the Hollingsworth instability associated to the vector-invariant form used with C grid finite difference methods (Hollingsworth, Kållberg, Renner and Burridge 1983), but this requires further investigation.

5.3. *Rotating compressible Euler equations*

For global atmosphere models, a standard approach is to solve the rotating compressible Euler equations, given by

$$u_t + (u \cdot \nabla)u + 2\Omega \times u + c_p\theta\nabla\Pi + g\hat{k} = 0, \tag{5.17}$$

$$\theta_t + u \cdot \nabla\theta = 0, \tag{5.18}$$

$$D_t + \nabla \cdot (uD) = 0, \tag{5.19}$$

$$\Pi = E(\theta, D), \tag{5.20}$$

where θ is the potential temperature, Π is the Exner pressure, D is now the density for three-dimensional models, c_p is the specific heat at constant pressure (a constant parameter in the ideal gas law) and E is a prescribed function describing the thermal equation of state relating Π, D and θ. This form of the equations is known as the 'theta-Pi' formulation. Other thermodynamic formulations make use of pressure and temperature directly, or other combinations of variables, but we do not discuss them here. For simplicity we consider boundary conditions $u \cdot n = 0$ on the bottom and top boundaries of the domain, although representations of the top of the atmosphere can be rather more complicated (since the real atmosphere has a

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density that decreases with height until it is so low that assumptions underlying the fluid dynamics model do not hold).

A compatible finite element formulation of the compressible Euler equations uses $u \in \mathbb{W}_h^2$, $D \in \mathbb{W}_h^3$ and $\theta \in \mathbb{W}_h^\theta$. Either Π is solved as an independent variable in $\mathbb{W}_h^3$, with the equation of state being projected into $\mathbb{W}_h^3$, or Π can just be replaced by $E(\theta, D)$ in the velocity equation, leading to a system for u, θ and D.

Natale *et al.* (2016) proposed a formulation using (4.19) as the transport scheme for velocity, upwind discontinuous Galerkin for density transport and the hybrid scheme for potential temperature used in Yamazaki *et al.* (2017). The main additional challenge is the discretization of the pressure gradient term $-\theta\nabla\Pi$ (which is scaled by c_p). In Yamazaki *et al.* (2017), the pressure gradient ∇p was integrated by parts, but this is more complicated in the compressible Euler case because of the presence of $\theta \in \mathbb{W}_h^\theta$, which can have discontinuities in the horizontal direction across vertical facets. We need to integrate by parts because Π is discontinuous, whether it is an independent variable in $\mathbb{W}_h^3$ or the evaluation of $E(D, \theta)$ (since $D \in \mathbb{W}_h^3$ is discontinuous). Natale *et al.* (2016) proposed applying integration by parts separately in each cell e for this term, obtaining

$$\int_e \nabla \cdot (w\theta)\Pi \,\mathrm{d}x - \int_{\partial e} \theta w \cdot n\{\Pi\} \,\mathrm{d}S \quad \text{for all } w \in \mathbb{W}_h^2(e), \tag{5.21}$$

where $\{\Pi\}$ is the average value of Π between the inside and the outside of e (since Π takes two values on ∂e). Summing this over all cells gives

$$\langle \nabla_h \cdot (w\theta), \Pi\rangle - \langle\!\langle [\![w\theta]\!], \{\Pi\} \rangle\!\rangle_\Gamma \quad \text{for all } w \in \mathbb{W}_h^2(\Omega), \tag{5.22}$$

where $\{\Pi\}$ is now defined as $(\Pi^+ + \Pi^-)/2$. Again, analogously to (5.7)–(5.8), a semi-implicit time-stepping scheme can be used, this time built around a linearization about a state of rest with $u = 0$, $\theta = \bar{\theta}$ and $\Pi = \bar{\Pi}$. These reference profiles vary in the vertical only, or – following the ENDGame approach (Wood *et al.* 2014) – the values of $\bar{\theta}$ and $\bar{\Pi}$ can be used from θ and Π at the previous time-step, but whilst neglecting their horizontal derivatives in the linearization to facilitate efficient solution. Finally, we neglect horizontal derivatives of $\Delta\theta$ appearing in the $\Delta\theta\nabla\bar{\Pi}$ term, for the same reason. This results in the following linear iteration, presented in Gibson (2019) (and used for the numerical results in Natale *et al.* 2016):

$$\begin{aligned} &\langle w, \Delta u\rangle + \frac{\Delta t}{2}\langle w, 2\Omega \times \Delta u\rangle \\ &- \frac{c_p \Delta t}{2}\langle \nabla_h \cdot (\bar{\theta} w), \Delta\Pi\rangle + \frac{c_p \Delta t}{2}\langle\!\langle [\![\bar{\theta} w]\!], \{\Delta\Pi\} \rangle\!\rangle_\Gamma \\ &- \frac{c_p \Delta t}{2}\langle \nabla \cdot (\hat{k}\Delta\theta\theta w \cdot \hat{k}), \bar{\Pi}\rangle = -R_u[w], \quad w \in \mathbb{W}_h^2, \end{aligned} \tag{5.23}$$

$$\langle \gamma, \Delta\theta\rangle + \frac{\Delta t}{2}\left\langle \gamma, \frac{\partial \bar{\theta}}{\partial z}\Delta u \cdot \hat{k}\right\rangle = -R_\theta[\gamma], \quad \gamma \in \mathbb{W}_h^\theta, \tag{5.24}$$

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$$\langle \phi, \Delta D\rangle - \frac{\Delta t}{2}\langle \nabla_h \phi, \bar{D}\Delta u\rangle + \frac{\Delta t}{2}\langle\!\langle [\![\phi \Delta u]\!], \{\bar{D}\}\rangle\!\rangle_\Gamma = -R_D[\phi], \quad \phi \in \mathbb{W}_h^3, \tag{5.25}$$

$$\Delta\Pi = \frac{\partial E}{\partial \theta}\Delta\theta + \frac{\partial E}{\partial D}\Delta D, \tag{5.26}$$

for the iterative updates $(\Delta u, \Delta\theta, \Delta D) \in \mathbb{W}_h^2 \times \mathbb{W}_h^\theta \times \mathbb{W}_h^3$ to $(u^{n+1}, \theta^{n+1}, D^{n+1})$. Alternatively, as was done in Melvin *et al.* (2019), we can add $\Delta\Pi \in \mathbb{W}_h^3$ to the list of independent variables and replace (5.26) with

$$\langle \alpha, \Delta\Pi\rangle = \left\langle \alpha, \frac{\partial E}{\partial \theta}\Delta\theta + \frac{\partial E}{\partial D}\Delta D \right\rangle \quad \text{for all } \alpha \in \mathbb{W}_h^3. \tag{5.27}$$

Melvin *et al.* (2019) adopted a hybrid approach, using finite volume methods to approximate the transport terms in a discretization otherwise built using compatible finite element methods.

5.4. *Iterative solver strategies*

Now we focus on the iterative solver strategies for these linear implicit systems. In all of the strategies we discuss here, the temperature $\Delta\theta$ is first (approximately) eliminated following our description of the approach to incompressible Boussinesq equations discussed above. This leads to the system

$$\begin{aligned} &\langle w, \Delta u\rangle + \frac{\Delta t}{2}\langle w, 2\Omega \times \Delta u\rangle \\ &- \frac{c_p \Delta t}{2}\langle \nabla\cdot(\bar{\theta} w), \Delta\Pi\rangle + \frac{c_p \Delta t}{2}\langle\!\langle [\![\bar{\theta} w]\!], \{\Delta\Pi\}\rangle\!\rangle_\Gamma \\ &- \frac{c_p \Delta t}{2}\langle \nabla\cdot(\hat{k}\Delta\theta\theta w\cdot\hat{k}), \bar{\Pi}\rangle = -R_u[w], \quad w \in \mathbb{W}_h^2, \end{aligned} \tag{5.28}$$

$$\langle \phi, \Delta D\rangle - \frac{\Delta t}{2}\langle \nabla_h \phi, \bar{D}\Delta u\rangle + \frac{\Delta t}{2}\langle\!\langle [\![\phi \Delta u]\!], \{\bar{D}\}\rangle\!\rangle_\Gamma = -R_D[\phi], \quad \phi \in \mathbb{W}_h^3, \tag{5.29}$$

$$\Delta\theta = -\frac{\Delta t}{2}\bar{\theta}\Delta u\cdot\hat{k} + r_\theta, \tag{5.30}$$

$$\Delta\Pi = \frac{\partial E}{\partial \theta}\Delta\theta + \frac{\partial E}{\partial D}\Delta D, \tag{5.31}$$

for $(\Delta u, \Delta D) \in \mathbb{W}_h^2 \times \mathbb{W}_h^3$, where $r_\theta \in \mathbb{W}_h^\theta$ such that

$$\langle r_\theta, \gamma\rangle = R_\theta[\gamma] \quad \text{for all } \gamma \in \mathbb{W}_h^\theta. \tag{5.32}$$

In other words, r_θ is the L^2 Riesz representer of R_θ. Mitchell and Müller (2016) proposed solving this reduced system using GMRES with a Schur complement preconditioner, using an approximate Schur complement formed from the lumped velocity mass matrix (and setting $\Omega = 0$). This was incorporated into a horizontal multigrid scheme (coarsening the mesh in the horizontal but not the vertical) using line smoothers (direct solves neglecting horizontal coupling between columns) for the approximate Schur complement on the levels. This combination of horizontal

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multigrid and vertical line smoothers is necessary because of the small aspect ratio of the atmosphere, and scalable parallel performance was observed over a large range of resolutions. This solve approach was successfully implemented in the Met Office system by Maynard, Melvin and Müller (2020), using the discretization approach of Melvin *et al.* (2019).

There is an alternative solution approach that has been applied to compatible discretizations of elliptic problems since the mid-twentieth century: hybridization. In hybridization, the continuity constraints of the $H(\mathrm{div})$ space are relaxed, and enforced through Lagrange multipliers as part of the solution formulation. The Lagrange multiplier space Tr, known as the trace space since it is supported only on cell facets, is chosen to match the $H(\mathrm{div})$ space when restricted to a facet and dotted with the normal component. This means that it is discontinuous between facets that meet at a vertex in two dimensions, or at an edge or vertex in three dimensions. For example, the hybridizable formulation of (5.7)–(5.8) seeks

$$(\Delta u, \Delta D, \lambda) \in \hat{\mathbb{V}}_h^1 \times \mathbb{V}_h^2 \times \mathrm{Tr}\big(\mathbb{V}_h^1\big) \tag{5.33}$$

such that

$$\begin{aligned} \langle w, \Delta u\rangle + \frac{\Delta t}{2}\langle w, f\Delta u^{\perp}\rangle & \\ -\frac{\Delta t}{2}\langle \nabla\cdot w, g\Delta u\rangle + \langle\!\langle [\![w]\!], \lambda\rangle\!\rangle_{\Gamma} &= -\tilde{R}_u[w] \quad \text{for all } w \in \hat{\mathbb{V}}_h^1, \qquad (5.34)\\ \left\langle \phi, \Delta D + \frac{H\Delta t}{2}\nabla\cdot\Delta u\right\rangle &= -R_D[\phi] \quad \text{for all } \phi \in \mathbb{V}_h^2, \qquad (5.35)\\ \langle\!\langle \gamma, [\![\Delta u]\!]\rangle\!\rangle_{\Gamma} &= 0 \quad \text{for all } \gamma \in \mathrm{Tr}(\mathbb{V}_h^1), \qquad (5.36) \end{aligned}$$

where

$$\tilde{R}_u[w] = R_u[w] \quad \text{for all } w \in \mathbb{V}_h^1. \tag{5.37}$$

To see that this is an equivalent formulation to (5.7)–(5.8), note that $\hat{\mathbb{V}}_h^1 \subset \mathbb{V}_h^1$, so we may choose $w \in \mathbb{V}_h^1$ in (5.34). In that case, the λ term vanishes because $[\![w]\!] = 0$, and we recover 5.7. Further, (5.36) ensures that $u \in \mathbb{V}_h^1$ at the solution, since taking $\gamma = [\![\Delta u]\!]$ implies that $[\![\Delta u]\!] = 0$ in $L^2(\Gamma)$; we note that

$$\mathbb{V}_h^1(\Omega) = \big\{u \in \hat{\mathbb{V}}_h^1(\Omega) \colon \|[\![u]\!]\|_{L^2(\Gamma)} = 0\big\}. \tag{5.38}$$

The advantage of this formulation is that Δu and ΔD can now both be eliminated elementwise, leading to a sparse system for λ; the reduced system is referred to as the hybridized system. This is possible because we can take w and ϕ supported in only one cell, and then given λ, we can solve for Δu and ΔD independently in each cell (this is referred to as the local solver). Material discussing the well-posedness of the hybridized system is surveyed in Boffi *et al.* (2013), along with postprocessing techniques for obtaining improved approximations using λ. A non-rigorous intuitive explanation for this is that λ gives an approximation of

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ΔD evaluated on facets, and hence the hybridized equation has properties of an approximation to the Helmholtz equation satisfied by ΔD after eliminating Δu from the linear PDE. This idea is built upon in Cockburn and Gopalakrishnan (2004), which provides an explicit weak form characterization of the hybridized method (including the non-symmetric term here containing $\Omega \times u$ is a straightforward extension of that work). This idea was used to demonstrate smoothing properties of standard iterative methods in Gopalakrishnan (2003) and a convergent multigrid scheme in Gopalakrishnan and Tan (2009). Gibson, Mitchell, Ham and Cotter (2020) applied the hybridization technique to the linear compressible Boussinesq equations, which are a minor modification of the linearization of the incompressible Boussinesq equations described above, incorporating linear acoustic waves.

This strategy cannot be applied to (5.28)–(5.31), because the averaging $\{\Delta\Pi\}$ of Π on facets couples the values of $\Delta\Pi$ between cells (and so there is no local solver). Gibson (2019) proposed a modification to address this, in which we seek $(\Delta u, \Delta D, \lambda) \in \hat{\mathbb{W}}_h^2 \times \mathbb{W}_h^3 \times \mathrm{Tr}(\mathbb{W}_h^2)$ such that

$$\begin{aligned}
&\langle w, \Delta u\rangle + \frac{\Delta t}{2}\langle w, 2\Omega \times \Delta u\rangle \\
&- \frac{c_p \Delta t}{2}\langle \nabla_h \cdot (\bar{\theta} w), \Delta\Pi\rangle + \frac{c_p \Delta t}{2}\langle\!\langle [\![\bar{\theta} w]\!], \lambda\rangle\!\rangle_\Gamma \\
&- \frac{c_p \Delta t}{2}\langle \nabla \cdot (\hat{k}\Delta\theta\theta w \cdot \hat{k}), \bar{\Pi}\rangle \\
&+ \underbrace{\frac{c_p \Delta t}{2}\langle\!\langle [\![\hat{k}\Delta\theta\theta w \cdot \hat{k}]\!], \{\Pi\}\rangle\!\rangle_{\Gamma_H}}_{\star} = -R_u[w], \quad w \in \hat{\mathbb{W}}_h^2, \qquad (5.39)
\end{aligned}$$

$$\langle \phi, \Delta D\rangle - \frac{\Delta t}{2}\langle \nabla\phi, \bar{D}\Delta u\rangle + \frac{\Delta t}{2}\langle\!\langle [\![\phi \Delta u]\!], \{\bar{D}\}\rangle\!\rangle_\Gamma = -R_D[\phi], \quad \phi \in \mathbb{W}_h^3, \qquad (5.40)$$

$$\langle\!\langle \gamma, [\![u]\!]\rangle\!\rangle_\Gamma = 0, \quad \gamma \in \mathrm{Tr}(\mathbb{W}_h^2), \qquad (5.41)$$

$$\Delta\theta = -\frac{\Delta t}{2}\bar{\theta}\Delta u \cdot \hat{k}, \qquad (5.42)$$

$$\Delta\Pi = \frac{\partial E}{\partial \theta}\Delta\theta + \frac{\partial E}{\partial D}\Delta D, \qquad (5.43)$$

where Γ_H is the set of horizontal faces between cells in the same vertical column. Here, the idea is that λ is an approximation of $c_p \Delta t \Delta\Pi/2$ on mesh facets. This system is not equivalent to (5.28)–(5.31), though. Note the addition of the term indicated with $\star$. This term vanishes when $w \in \mathbb{W}_h^2$, so it does not change the solution, but it was found that without it, iterative solvers do not perform well; it appears to be required for the coercivity of the solution. This system has not been analysed yet, but it was demonstrated to produce comparable results to standard test cases when applied to the full nonlinear compressible Euler equations. Scalable multigrid behaviour for the hybridized system was also demonstrated.

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Bendall *et al.* (2020) extended this solver approach to the compressible Euler equations with moisture, where the mass lumping approach was found not to work well when RT_1 spaces were used. Betteridge *et al.* (2022) showed that this hybridization approach produces scalable results for the Met Office formulation of Melvin *et al.* (2019).

5.5. *Computing hydrostatic balanced states*

The hybridization approach also provides a useful way to solve for hydrostatic balanced states, satisfying

$$-\langle \nabla\cdot(\theta w),\Pi\rangle = \langle w\cdot\hat{k},g\rangle - \langle\!\langle w\cdot n,\Pi_0\rangle\!\rangle \quad \text{for all } w\in \mathring{\mathbb{W}}_h^{2,V}. \tag{5.44}$$

Following the technique of Natale *et al.* (2016) previously discussed, for given $\theta\in\mathbb{W}_h^\theta$, we seek $(v,D)\in\mathbb{W}_h^2\times\mathbb{W}_h^3$ such that

$$\langle w,v\rangle - \langle \nabla\cdot(\theta w),\Pi\rangle = \langle w\cdot\hat{k},g\rangle - \langle\!\langle w\cdot n,\Pi_0\rangle\!\rangle \quad \text{for all } w\in \mathring{\mathbb{W}}_h^{2,V}, \tag{5.45}$$

$$\langle \phi,\nabla\cdot v\rangle = 0 \quad \text{for all } \phi\in\mathbb{W}_h^3, \tag{5.46}$$

$$\Pi = E(\theta,D), \tag{5.47}$$

which is independent between columns. An equivalent hybridizable formulation seeks $(v,D)\in\mathbb{W}_h^2\times\mathbb{W}_h^3$ such that

$$\langle w,v\rangle - \langle \nabla\cdot(\theta w),\Pi\rangle + \langle\!\langle [\![w]\!],\lambda\rangle\!\rangle_\Gamma = \langle w\cdot\hat{k},g\rangle - \langle\!\langle w\cdot n,\Pi_0\rangle\!\rangle \quad \text{for all } w\in \hat{\mathbb{W}}_h^{2,V}, \tag{5.48}$$

$$\langle \phi,\nabla\cdot v\rangle = 0 \quad \text{for all } \phi\in\mathbb{W}_h^3, \tag{5.49}$$

$$\langle\!\langle \gamma,[\![v]\!]\rangle\!\rangle_\Gamma = 0 \quad \text{for all } \gamma\in \mathrm{Tr}\big(\mathbb{W}_h^{2,V}\big), \tag{5.50}$$

$$\Pi = E(\theta,D), \tag{5.51}$$

where Γ now includes the bottom boundary (but not the top), and $\mathrm{Tr}(\mathbb{W}_h^{2,V})$ is only supported on horizontal facets between neighbouring cells in the same column. This can be solved using Newton's method, with solution of the Jacobian system via the hybridized system for $\delta\lambda$.

5.6. *Monolithic solvers*

One more recent solver approach has been investigated in numerical experiments in Cotter and Shipton (2022), who used a similar suite of discretizations to that of Natale *et al.* (2016), with the exception of using edge stabilization for potential temperature instead of vertical SUPG. In this work, the fully nonlinear implicit midpoint rule is solved using Newton's method, and GMRES is applied to the coupled system for $\Delta u,\Delta\theta,\Delta D$ without elimination. The system is preconditioned by an additive Schwarz method, computing exact solutions of the Jacobian system restricted to overlapping columnar patches; each patch consists of the cells surrounding one vertical edge (excluding degrees of freedom attached to the vertical

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facets on the side boundaries of the patch). This scheme also requires further analysis, but was shown to produce mesh independent iteration counts in numerical experiments.

6. Variational discretizations

Variational discretizations are discretizations that are derived from a discrete Hamilton's principle. They were originally introduced in the setting of ordinary differential equations (ODEs), taking the name 'variational integrators', surveyed in Marsden and West (2001). The idea behind variational discretizations is that rather than discretizing the equations directly, we instead discretize the action functional from which the equations are derived. In the case of ODEs, this means replacing the time integral with a discrete quadrature rule involving the solution at discrete points in time. The discretization of the equations is then obtained by finding stationary points of the discretized Lagrangian.

The advantage of variational discretizations is that if the discretized action has symmetries, then these symmetries give rise to corresponding conserved quantities via (the discrete) Noether's theorem. In the context of variational integrators for mechanical systems, this yields discrete conservation of momentum and angular momentum, for example. Further, after Legendre transformation the discrete time-stepping map is symplectic, leading to the conservation (up to exponentially small terms in Δt) of a modified energy/Hamiltonian obtained through backward error analysis (Hairer, Wanner and Lubich 2006, Hairer, Lubich and Wanner 2003, Leimkuhler and Reich 2004, Sanz-Serna 1992).

In principle, the variational discretization approach can be extended directly to partial differential equations by simply discretizing the action functional in space as well as in time (or one may consider spatial semidiscretization by discretizing in space only, as we shall mostly do here). For fluid dynamics, the situation is more challenging, because the underlying variational principle is defined in terms of the Lagrangian flow map rather than the Eulerian quantities. This is discussed in the following subsection.

6.1. Hamilton's principle for fluid dynamics: continuous theory

The Lagrangian flow map is treated formally (we avoid discussions of smoothness, etc.) as a diffeomorphism $\chi(\cdot, t)\colon \Omega_0 \to \Omega$, mapping labels in a configuration space Ω_0 to fluid particle locations at time t in the physical domain Ω. We have a time-t family of maps.[2] The variational formulation then follows by writing an action as an integral over Ω_0, and variations in χ are considered subject to the usual endpoint conditions in time plus the requirement that χ be a diffeomorphism. Working with these Lagrangian flow maps is difficult both for theory and numerical computation;

[2] Here we use the notation $\chi(\cdot, t)$ to indicate the function $x \mapsto \chi(x, t)$ for given t.

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this was addressed by Arnold's geometric formulation in Eulerian variables for the incompressible Euler equations (Arnold 1966). For each $(x,t) \in \Omega \times [0,T]$, where T is the time interval over which the equations are being solved, $u(x,t)$ is a vector tangent to x at Ω.[3] For each t, we say that $u(\cdot,t) \in \mathfrak{X}(\Omega)$, the space of vector fields on Ω.

The formulation stems from the observation that the Eulerian velocity u satisfies

$$\frac{\partial}{\partial t}\chi = u \circ \chi, \tag{6.1}$$

where for functions of (x,t) we write $(u \circ \chi)(x,t) = u(\chi(x,t),t)$. To construct Hamilton's principle, we need to consider perturbations to χ that are still diffeomorphisms for each t. If we consider such a continuous two-parameter family of perturbed maps $\tilde{\chi}(x,t,\epsilon)$, with $\tilde{\chi}(x,t,\epsilon = 0) = \chi(x,t)$, then there exists a continuous family of vector fields $\tilde{w}(\cdot,t,\epsilon) \in \mathfrak{X}(\Omega)$ such that

$$\frac{\partial}{\partial \epsilon}\tilde{\chi} = \tilde{w} \circ \tilde{\chi}, \tag{6.2}$$

where we now extend the $\circ$ notation to the case of two parameters, ϵ and t, writing $(\tilde{w} \circ \tilde{\chi})(x,t,\epsilon) = \tilde{w}(\tilde{\chi}(x,t,\epsilon),t,\epsilon)$. Differentiating with respect to ϵ and evaluating at $\epsilon = 0$, we get the infinitesimally perturbed χ,

$$\delta\chi \coloneqq \frac{\partial}{\partial \epsilon}\bigg|_{\epsilon=0}\tilde{\chi} = w \circ \chi, \tag{6.3}$$

where $w(x,t) \coloneqq \tilde{w}(x,t,\epsilon = 0)$. Here $\delta\chi$ depends on the direction of perturbation in the parameter ϵ, so we always consider $\delta\chi$ being defined with respect to a particular choice of w. By differentiating (6.1) with respect to ϵ, we obtain

$$\begin{aligned}\delta\frac{\partial}{\partial t}\chi &= (\nabla u) \circ \chi \cdot \delta\chi + \delta u \circ \chi \\ &= (\nabla u) \circ \chi \cdot w \circ \chi + \delta u \circ \chi,\end{aligned} \tag{6.4}$$

where

$$\delta u \coloneqq \frac{\partial}{\partial \epsilon}\bigg|_{\epsilon=0}\frac{\partial}{\partial t}\chi \circ \chi^{-1}. \tag{6.5}$$

Similarly, by differentiating (6.3) with respect to t, we obtain

$$\begin{aligned}\frac{\partial}{\partial t}\delta\chi &= (\nabla w) \circ \chi \cdot \frac{\partial}{\partial t}\chi + \frac{\partial}{\partial t}w \circ \chi \\ &= (\nabla w) \circ \chi \cdot u \circ \chi + \frac{\partial}{\partial t}w \circ \chi.\end{aligned} \tag{6.6}$$

By subtracting (6.4) and (6.6), noting the symmetry of second derivatives and

[3] We have $u(x,t) \in \mathbb{R}^N$ for the case where Ω is an N-dimensional subset of $\mathbb{R}^N$, but in geophysical fluid dynamics we are also interested in solving problems where Ω is the surface of a sphere.

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composing with χ^{-1}, we obtain

$$\delta u = \frac{\partial}{\partial t} w + \underbrace{u \cdot \nabla w - w \cdot \nabla u}_{= [u,w]}. \tag{6.7}$$

Hence we have successfully related infinitesimal perturbations ('variations') in u to variations in χ entirely in terms of the Eulerian quantities u and w. Arnold used this calculation to derive the incompressible Euler equations by seeking $u \in \mathfrak{X}_{\mathrm{vol}}(\Omega)$ (the subspace of $\mathfrak{X}(\Omega)$ containing divergence-free vector fields), that extremize the reduced action functional

$$S = \int_0^T \int_\Omega \frac{1}{2} |u|^2 \, \mathrm{d}x \, \mathrm{d}t, \tag{6.8}$$

subject to endpoint conditions $u|_{t=0} = u_0$, $u|_{t=T} = u_T$ (for some chosen u_0 and u_T), and the boundary conditions $u \cdot n = 0$ on the boundary $\partial\Omega$ of the domain Ω, where n is the outward-pointing normal to $\partial\Omega$. If we perturb u subject to these conditions, this implies that $w_{t=0} = w_{t=T} = 0$.

Taking variations gives

$$\begin{aligned}
0 = \delta S &= \int_0^T \int_\Omega \delta u \cdot u \, \mathrm{d}x \, \mathrm{d}t \\
&= \int_0^T \int_\Omega \left(\frac{\partial}{\partial t} w + [u, w] \right) \cdot u \, \mathrm{d}x \, \mathrm{d}t \\
&= \int_0^T \int_\Omega w \cdot \left(-\frac{\partial}{\partial t} u - \nabla \cdot (u \otimes u) - \underbrace{(\nabla u)^\top u}_{= \frac{1}{2} \nabla |u|^2} \right) \mathrm{d}x \, \mathrm{d}t \\
&\quad + \int_0^T \int_{\partial\Omega} \underbrace{u \cdot n}_{=0} \, w \cdot u \, \mathrm{d}S \, \mathrm{d}t \\
&\quad + \left[\int_\Omega u \cdot \underbrace{w}_{=0} \, \mathrm{d}x \right]_{t=0}^{t=T} \qquad \text{for all } w \in \mathfrak{X}_{\mathrm{vol}}(\Omega),
\end{aligned} \tag{6.9}$$

where $(u \otimes u)_{ij} = u_i u_j$, and $(\nabla u)_{ij} = \partial u_i / \partial x_j$. This formally implies that

$$\mathbb{P} \left(\frac{\partial}{\partial t} u + u \cdot \nabla u \right) = 0, \tag{6.10}$$

where $\mathbb{P}$ is the L^2 projection onto divergence-free vector fields. In other words, there exists a pressure p such that

$$\frac{\partial}{\partial t} u + u \cdot \nabla u + \nabla p = 0, \tag{6.11}$$

which is the familiar form of the incompressible Euler equation (together with the divergence-free constraint $\nabla \cdot u = 0$).

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Besides the usual translational and rotational symmetries (assuming appropriate boundary conditions), the variational formulation has an additional particle relabelling symmetry, meaning that we can replace χ with $\chi \circ \psi$ for any diffeomorphism $\psi : \Omega_0 \rightarrow \Omega_0$ and the action remains invariant (in fact the value of u does not change). Physically this corresponds to the fact that the fluid physics is independent of the choice of label for a fluid particle (the label for a fluid particle at time t and position x_0 being $\chi^{-1}(x)$, i.e. $\chi(x_0, t) = x$). As discussed in many places (e.g. Morrison 1982, Salmon 1998, Shepherd 1990), this symmetry leads to conservation of circulation

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{C(t)} u \cdot \mathrm{d}x = 0, \tag{6.12}$$

for closed loops $C(t)$ that are being transported by the fluid velocity u.

The reduction from the flow map χ to the Eulerian velocity by Arnold was characterized in Holm, Marsden and Ratiu (1998) as Euler–Poincaré reduction by symmetry. In that work, this framework was extended to quantities that are advected by the flow, including densities solving the continuity equation, tracers solving the advection equation, etc., leading to the derivation of the full family of geophysical fluid dynamics models and beyond: quasigeostrophic approximations (Holm and Zeitlin 1998), complex fluids (Holm 2002, Gay-Balmaz and Ratiu 2009), vertical slice models (Cotter and Holm 2013*b*), pseudocompressible and anelastic approximations (Cotter and Holm 2014), the Boussinesq-alpha model (Badin, Oliver and Vasylkevych 2018) and models with moisture and irreversible processes (Gay-Balmaz 2019). The derivation of conservation laws associated with particle relabelling symmetries through Noether's theorem applied to this framework was presented in Cotter and Holm (2013*a*) and Cotter and Cullen (2019).

6.2. *Koopman representation: continuous theory*

The difficulty with adapting Hamilton's principle, as described above, to discretizations is that there does not exist a finite-dimensional subspace of flow maps that closes appropriately under composition. A solution to this, proposed by Pavlov *et al.* (2011), is to use the Koopman representation of flow maps. We shall only briefly describe their approach here, but will provide more detail about the extension to compatible finite elements shortly.

In the Koopman framework, flow maps χ in the group $\mathrm{Diff}(\Omega)$ of diffeomorphisms on Ω are represented by elements of $GL(L^2(\Omega))$, the invertible linear maps from $L^2(\Omega)$ to $L^2(\Omega)$. In particular, flow maps χ represented by linear maps $\rho_\chi \in GL(L^2(\Omega))$ are defined by $\rho_\chi \cdot a \equiv \rho_\chi(a) = a \circ \chi^{-1}$. Of course, there are many maps in $GL(L^2(\Omega))$ that cannot be written in this way, so there is not an isomorphism. In fact, the map defines a subgroup of $GL(L^2(\Omega))$, which we call $G(L^2(\Omega))$, which is isomorphic to the group $\mathrm{Diff}(\Omega)$.

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To specialize to incompressible flows, we use $GL_0(L^2(\Omega))$, defined as

$$GL_0(L^2(\Omega)) = \big\{\rho \in GL(L^2(\Omega)) \colon (\rho \cdot a, \rho \cdot b)_\Omega = (a, b)_\Omega \quad \text{for all } a, b, \in L^2(\Omega), \text{ and } \rho \cdot c = c \text{ for all } c \in \mathbb{R}\big\}. \tag{6.13}$$

The ρ_χ representation defines an isomorphism of a subgroup of $GL_0(L^2(\Omega))$, which we call $G_0(L^2(\Omega))$, to the group of volume preserving diffeomorphisms $\mathrm{Diff}_{\mathrm{vol}}(\Omega)$. The group $G_0(L^2(\Omega))$ was approximated in numerical discretizations of the incompressible Euler equations in Pavlov *et al.* (2011); the extension to the full diffeomorphism group was used in the extension to compressible models of geophysical fluid dynamics in Desbrun, Gawlik, Gay-Balmaz and Zeitlin (2014), Bauer and Gay-Balmaz (2017), Brecht *et al.* (2019) and Bauer and Gay-Balmaz (2019).

The Koopman representation also provides an isomorphism between the Lie algebra $\mathfrak{X}(\Omega)$, corresponding to vector fields on Ω, and a subspace of the Lie algebra $\mathfrak{gl}(L^2(\Omega))$, which we call $\mathfrak{g}(L^2(\Omega))$. For a one-parameter family $\chi_s \in \mathrm{Diff}(L^2(\Omega))$ of maps with $\chi_0 = \mathrm{Id}$ and

$$\frac{\mathrm{d}}{\mathrm{d}s}\Big|_{s=0} \chi_s = v, \tag{6.14}$$

we have

$$\frac{\mathrm{d}}{\mathrm{d}s}\Big|_{s=0} \rho_{\chi_s} a = \frac{\mathrm{d}}{\mathrm{d}s}\Big|_{s=0} \left(a \circ \chi_s^{-1}\right) := -L_v a = v \cdot \nabla a, \tag{6.15}$$

where L_v is called the *Lie derivative*. Corresponding definitions follow for the restrictions $\mathrm{Diff}(\Omega) \to \mathrm{Diff}_{\mathrm{vol}}(\Omega)$ and $GL(L^2(\Omega))$ to $GL_0(L^2(\Omega))$.

6.3. *Previous work on variational discretizations using Koopman representation*

Pavlov *et al.* (2011) used the Koopman representation to derive a discrete variational principle that considered finite subspaces $GL(V)$, where V is the space of cellwise constant functions defined on a mesh. The subset $G_h \subset GL(V)$ approximating the flow maps was identified as being generated by maps that only allow instantaneous fluxes between neighbouring cells (thus approximating the diffeomorphism property). These fluxes can be described within the framework of discrete exterior calculus (DEC) (Hirani 2003). The difficulty with trying to discretize this structure is that it is not possible to find a subset G_h that can be generated by a finite subspace of $\mathfrak{gl}(V)$. This was addressed by introducing a *non-holonomic constraint* on the time derivative of the flow map (and corresponding Koopman representative of $GL(V)$). Remarkably, Hamilton's principle under these constraints is still reducible (i.e. the $GL(V)$ elements can be eliminated in favour of their generating vector fields), leading to a discretization that can be solved entirely in terms of Eulerian velocities, yielding a spatial discretization that corresponds to a known marker-and-cell scheme when a structured grid of square cells is used. This spatial discretization is then combined with quadrature approximation in time to produce a fully discrete variational integrator for fluid dynamics.

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The principal goal of the variational discretization is to obtain schemes with discrete conservation laws. Before time discretization, the discrete action is invariant under time translations, leading to conservation of energy. Time discretization breaks this symmetry, but there is the potential to apply backward error analysis to obtain exponentially accurate conservation of a modified energy. Whilst numerical results from these variational schemes do exhibit long-time approximate energy conservation, as would be expected from this backward error analysis, it has not yet been adapted to the type of non-holonomic constraints occurring in this framework. The variational scheme also contains an echo of the circulation theorem. Instead of considering loops, we consider currents. These are objects dual to velocities, defined by the duality pairing

$$c[v] = \int_\Gamma v \cdot \mathrm{d}x \quad \text{for all } v \in \mathfrak{X}(\Omega), \tag{6.16}$$

for some curve Γ. Currents are transported by a flow map χ via $c \mapsto ((\nabla\chi)c) \circ \chi^{-1}$, allowing Kelvin's circulation theorem to be reformulated (in the case of incompressible Euler equations) as

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(((\nabla\chi)c) \circ \chi^{-1}\right)[u] = 0. \tag{6.17}$$

There is a discrete analogue of this formula when currents are approximated by objects dual to velocity fields on the discrete grid. These discrete currents can be considered to be loops that have been smoothed out over a finite area. This can be used to define a discrete circulation that is conserved along the solution, including the discrete-time solution. However, since the approximation of a discrete current to a continuous current corresponding to an advected loop gets noisier as time progresses, it is not clear how or whether these discrete conservation laws constrain the discrete fluid dynamics in the same way that circulation conservation does in the continuous case (which occurs through the link to Casimirs on the Hamiltonian side). This is another important open question about this framework.

6.4. Compatible finite element variational discretization of incompressible flow

Inspired by the observation of Dmitry Pavlov that one could extend this framework to other discretization methods by simply selecting a discrete space for velocity fields and a discrete approximation of their Lie group action on scalar fields, and noting the links between DEC and FEEC, Natale and Cotter (2018) developed such an extension to compatible finite element methods for the incompressible Euler case. In this case, we use the space of velocity fields $\mathring{W}_h^r$ defined by

$$\mathring{W}_h^r = \left\{u \in W_h^r : \nabla \cdot u = 0,\ u \cdot n|_{\partial\Omega} = 0\right\}, \tag{6.18}$$

where W_h^r is a degree r BDM or RT space (they both have the same divergence-free subspace so the distinction is not important here). For the discrete Koopman representation of the flows generated by these velocity fields, we select V_h^s, the space

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of discontinuous piecewise polynomials of degree s. Following the discrete Lie derivative framework (the Eulerian version in particular) of Heumann and Hiptmair (2011), given $u \in \mathring{W}_h^r$, we define the discrete advection operator $X_u \in \mathfrak{gl}(V_h^s)$ defined by

$$\langle X_u a, b\rangle = -\langle a, \nabla\cdot(ub)\rangle + \langle\!\langle [\![au]\!], \{b\}\rangle\!\rangle_\Gamma \quad \text{for all } a, b \in V_h^s, \tag{6.19}$$

where $\{b\} = (b^+ + b^-)/2$. This is a centred approximation of the advection operator on V_h^s, meaning that X_u is linear in u (an upwinded approximation would break this).

To develop the non-holonomic constraint that enforces a dynamics that converges to fluid motion by diffeomorphism, we seek a Koopman representation of a time-dependent flow map $\hat{\chi}(\cdot, t) \in G(V_h^s)$ that transports advected tracers according to $a = \hat{\chi}\cdot a_0$. If we require that all such advected tracers satisfy the equation

$$\frac{\mathrm{d}}{\mathrm{d}t} a + X_u a_0 = 0, \tag{6.20}$$

for some time-dependent velocity field $u \in \mathring{W}_h^r$, then we obtain the *non-holonomic constraint* on $\hat{\chi}$ that

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\chi}_h \cdot a + X_u\hat{\chi}\cdot a = 0 \quad \text{for all } a \in V_h, \tag{6.21}$$

for some $X_u \in \mathfrak{gl}(V_h^s)$, that is,

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\chi} + X_u\hat{\chi} = 0. \tag{6.22}$$

This constraint describes the approximation $\hat{\chi} \in G_h$ to the Koopman representation $\hat{\chi} \in G(L^2(\Omega))$ of the flow map χ. It is non-holonomic because it constrains the time derivative of $\hat{\chi}$, not $\hat{\chi}$ itself, and this constraint cannot be integrated to obtain such a constraint $F(\hat{\chi}) = 0$. This is because the subspace $S_h^r(V_h^s) \subset \mathfrak{gl}(V_h^s)$ defined by the image of the map $u \in \mathring{W}_h^r \mapsto X_u$ is not closed under Lie brackets. In other words $[X_u, X_v]$ is not guaranteed to be in $S_h^r(V_h^s)$ for all $X_u, X_v \in S_h^r(V_h^s)$.

Natale and Cotter (2018) proved that if $r \geq s$, then the map between $u \in W_h^r$ and $X_u \in S_h^r(V_h^s) \subset \mathfrak{gl}(V_h^s)$ is an isomorphism. Gawlik and Gay-Balmaz (2021*b*) took this further, by considering the extension of X_u to the whole of $H(\mathrm{div}) \cap L^p(\Omega)^n$ (with some $p > 2$; this technicality ensures the existence of traces on individual facets), using the same formula (6.19). They considered the space $\hat{S}_h(V_h^s) \subset \mathfrak{gl}(V_h^s)$, defined by

$$\hat{S}_h(V_h^s) = \{X_u : u \in H(\mathrm{div}) \cap L^p(\Omega)^n\}, \tag{6.23}$$

and proved that $\hat{S}_h(V_h^s)$ is isomorphic to RT^{2r} (via the isomorphism $u \mapsto X_u$). This shows that subspaces of RT^{2r} are a necessary choice for W_h^r. When discontinuous finite element spaces are chosen for V, the compatible finite element framework is thus a necessity rather than a choice.

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To continue the derivation of the discrete incompressible Euler equations, we need to form the Lagrangian, which is just the kinetic energy. Defined in terms of the original flow map, the undiscretized Lagrangian is

$$\int_\Omega \frac{1}{2}|u|^2 \,\mathrm{d}x. \tag{6.24}$$

In the finite element framework, we need to write this Lagrangian as a functional of $X_u \in S_h(V_h^s)$, but we need to be able to recover u from X_u to substitute into the kinetic energy. As proposed by Dmitry Pavlov, Natale and Cotter (2018) obtained an approximation to this Lagrangian by applying X_u to each of the Cartesian coordinates, that is,

$$u = \overline{X_u} = \sum_{i=1}^{N} X_u(x_i) e_i, \tag{6.25}$$

where e_i is the unit vector in the direction of increasing coordinate x_i.[4] This presentation assumes a Cartesian metric, and suitable changes need to be made for solution of the equations on manifolds such as the surface of a sphere.

To properly define Hamilton's principle, we need to define the Lagrangian on the whole tangent bundle $TG_h(V)$ of $G_h(V)$, consisting of pairs $((\partial/\partial t)\hat{\chi}, \hat{\chi})$ with $\hat{\chi} \in G_h(V)$. Thus we extend the definition of the 'overbar map' (6.25) to the whole of $\mathfrak{gl}(V_h)$,

$$\overline{\xi} = \sum_{i=1}^{N} e_i \xi \cdot x_i \quad \text{for all } \xi \in \mathfrak{gl}(V_h), \tag{6.26}$$

and write the Lagrangian $L_h : TG_h(V) \to \mathbb{R}$ as

$$L_h = \int_\Omega \frac{1}{2} \left\| \overline{\left(\frac{\partial}{\partial t}\hat{\chi} \circ \hat{\chi}^{-1} \right)} \right\|^2 \mathrm{d}x. \tag{6.27}$$

We can write this as a reduced Lagrangian on $\mathfrak{gl}(V_h^s)$:

$$\ell_h[X] = \int_\Omega \frac{1}{2} \|\overline{X}\|^2 \,\mathrm{d}x. \tag{6.28}$$

The Lagrange–D'Alembert principle (Hamilton's principle with non-holonomic constraints) seeks $\hat{\chi}$ with $(\partial/\partial t)\hat{\chi}$ satisfying (6.22) such that

$$\delta \int_0^T L_h\left(\frac{\partial}{\partial t}\hat{\chi}, \hat{\chi} \right) \mathrm{d}t = 0, \tag{6.29}$$

for all variations $\delta\hat{\chi}$ satisfying

$$\delta\hat{\chi} + X_w \hat{\chi} = 0, \tag{6.30}$$

[4] In fact, this was used to prove the isomorphism between X_u and u.

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for some time-dependent $w \in \mathring{W}_h^r$. If we have a Lagrangian (such as (6.27)) that is reducible by right action, that is,

$$L_h\left(\frac{\partial}{\partial t}\hat{\chi}, \hat{\chi}^{-1}\right) = \ell_h\left(\frac{\partial}{\partial t}\hat{\chi} \circ \hat{\chi}^{-1}\right), \tag{6.31}$$

then we can perform Euler–Poincaré reduction, taking care with the non-holonomic constraint. This proceeds much as in the unapproximated case described above, as follows. If we have g such that

$$\frac{\partial}{\partial t}\hat{\chi} + X\hat{\chi} = 0,\ \delta\hat{\chi} + Y\hat{\chi} = 0, \tag{6.32}$$

for $X, Y \in \mathfrak{gl}(V_h^s)$, then calculations identical to the above lead to

$$(\delta X)\hat{\chi} + XY\hat{\chi} - \frac{\partial}{\partial t}Y\hat{\chi} - YX\hat{\chi} = 0, \tag{6.33}$$

that is,

$$\delta X = \frac{\partial}{\partial t}Y + [X, Y], \tag{6.34}$$

where $[X, Y] = XY - YX$ is the usual commutator for linear operators. Thus the Lagrange–D'Alembert principle can be reduced to the corresponding reduced D'Alembert principle, as follows. Find $X \in \mathfrak{gl}(V_h^s)$ subject to the constraint

$$X = X_u, \tag{6.35}$$

for some $u \in \mathring{W}_h^r$, such that

$$\delta \int_0^T \ell_h(X)\,\mathrm{d}t = 0, \tag{6.36}$$

for variations of the form (6.34) for all time-dependent $Y \in \mathfrak{gl}(V_h^s)$, subject to the constraint $Y = X_w$ for some time-dependent $w \in \mathring{W}_h^r$. The non-closure of $S_h^r(V_h^s)$ under Lie brackets together with the appearance of the Lie bracket in (6.34) is the reason why we defined a Lagrangian $TG_h(V)$ and not just for $\hat{\chi}$ satisfying the constraint.[5] From this reduced principle, we can derive the Euler–Poincaré–D'Alembert equation

$$\left\langle \frac{\mathrm{d}}{\mathrm{d}t}\frac{\delta l_h}{\delta X}, Y \right\rangle + \left\langle \frac{\delta l_h}{\delta X}, [X, Y] \right\rangle = 0, \tag{6.37}$$

for all Y satisfying (6.34), where

$$\left\langle \frac{\delta l_h}{\delta X}, Y \right\rangle := \delta l_h[X; \delta X] = \lim_{\epsilon \to 0} \frac{L[X + \epsilon\delta X] - L[X]}{\epsilon}. \tag{6.38}$$

[5] In fact, it is only necessary to define the reduced Lagrangian ℓ_h for $X = X_u$ and $X = [X_u, X_v]$ for $u, v \in \mathring{W}_h^r$. This is how the problem was approached for the discrete exterior calculus formulation Pavlov *et al.* (2011). However, the finite element framework and the bar map makes it easy enough to extend to the whole of $\mathfrak{gl}(V_h^s)$.

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For our reduced Lagrangian (6.28), we have

$$\left\langle \frac{\delta \ell_h}{\delta X}, \delta X \right\rangle = \delta \ell_h[X; \delta X] = \langle \delta \bar{X}, \bar{X} \rangle = \langle \delta \bar{X}, \bar{X} \rangle \quad \text{for all } \delta X \in \mathfrak{gl}(V_h^s). \tag{6.39}$$

This means that solving (6.37) is equivalent to finding $A_h \in S_h^r(V_h)$ such that

$$\left\langle \frac{\mathrm{d}}{\mathrm{d}t} \bar{A}_h, \bar{B}_h \right\rangle_\Omega + \left\langle \bar{A}_h, \overline{[A_h, B_h]} \right\rangle_\Omega = 0, \tag{6.40}$$

for all $B_h \in S_h^r(V_h)$, where $[\cdot, \cdot]$ is the commutator bracket for linear operators. Natale and Cotter (2018) then showed that (6.37) is equivalent to finding $u \in \mathring{W}_s$ such that

$$\left\langle \frac{\partial}{\partial t} u, v \right\rangle_\Omega + \langle X_u u, v \rangle = 0 \quad \text{for all } v \in \mathring{W}_h^r, \tag{6.41}$$

where $X_u : \mathring{W}_h^r \to \mathring{W}_h^r$ is defined as

$$\langle X_u a, b \rangle = \langle a, \nabla_h \times (u \times b) - u \nabla \cdot b \rangle + \langle\!\langle \{u\}, [\![n \times (u \times b)]\!] \rangle\!\rangle_\Gamma. \tag{6.42}$$

Surprisingly, given all of the complexity in the formulation, this takes the form of a conventional finite element approximation without ever needing to calculate X_u. Some further manipulation shows that this discretization is in fact identical to the centred flux discretization described in Guzmán, Shu and Sequeira (2017), which emerged around the same time (but without the variational derivation).

6.5. *Compatible finite element discretization for compressible fluids*

The framework was extended to compressible fluid equations in Gawlik and Gay-Balmaz (2021*b*), which applied the programme of Desbrun *et al.* (2014) and Bauer and Gay-Balmaz (2019) to the compatible finite element case. This involves the introduction of advected quantities such as temperature (which satisfies a scalar advection equation) and density (which satisfies a continuity equation). In the unapproximated equations, this enables us to treat Lagrangians of the form

$$L\left(\frac{\partial \chi}{\partial t}, \chi \right) = \ell(u, a_1, a_2, \ldots, a_n), \tag{6.43}$$

where a_i are advected quantities satisfying

$$\frac{\partial}{\partial t} a_i + \mathcal{L}_u a_i = 0, \tag{6.44}$$

where $\mathcal{L}_u$ is a Lie derivative of an appropriate type, e.g. for advected scalars a,

$$\mathcal{L}_u a = u \cdot \nabla a, \tag{6.45}$$

as before, whilst for advected densities D,

$$\mathcal{L}_u D = \nabla \cdot (uD). \tag{6.46}$$

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In that case, Hamilton's principle leads to the Euler–Poincaré equation with advected quantities (Holm *et al.* 1998)

$$\frac{\partial(\delta l/\delta u)}{\partial t} + u \cdot \nabla \frac{\delta l}{\delta u} + (\nabla u)^{\top} \frac{\delta l}{\delta u} = \sum_i a_i \diamond \frac{\delta l}{\delta a_i}, \tag{6.47}$$

where the diamond operator $\diamond$ is defined by

$$\left\langle a_i \diamond \frac{\delta l}{\delta a_i}, w \right\rangle = -\left\langle \mathcal{L}_w a_i, \frac{\delta l}{\delta a_i} \right\rangle, \tag{6.48}$$

for all vector fields w. This allows for the relaxation to arbitrary diffeomorphisms instead of volume preserving ones, and enables the variational derivation of the full range of compressible fluid models arising in geophysical fluid dynamics and beyond. In particular, the incompressible Euler equation can be recovered by introducing a Lagrange multiplier (the pressure) to enforce constant density D.

In the Koopman operator framework, discrete advected densities $D \in V_h^s$ are treated by defining their transport equation as being dual to that of scalar functions $f \in V_h^s$, that is, if $f = \hat{\chi} f_0 \in V_h^s$,

$$\langle D, f \rangle = \langle D_0, f_0 \rangle. \tag{6.49}$$

Hence

$$\begin{aligned} 0 = \frac{\partial}{\partial t}\langle D, f\rangle &= \left\langle \frac{\partial}{\partial t} D, f \right\rangle + \left\langle D, \frac{\partial}{\partial t} f \right\rangle \\ &= \left\langle \frac{\partial}{\partial t} D, f \right\rangle - \langle D, Xf \rangle. \end{aligned} \tag{6.50}$$

Therefore we conclude that

$$\left\langle \frac{\partial}{\partial t} D, \phi \right\rangle - \langle X^* D, \phi \rangle = 0 \quad \text{for all } \phi \in V_h^s, \tag{6.51}$$

where

$$X = \left(\frac{\partial}{\partial t} g \right) \circ g^{-1} \in \mathfrak{gl}\big(V_h^s\big). \tag{6.52}$$

When X satisfies the non-holonomic constraint $X = X_u$ for some $u \in W_h^r$, this becomes

$$\begin{aligned} \left\langle \frac{\partial}{\partial t} D, \phi \right\rangle &= \langle X_u^* D, \phi \rangle = \langle D, X_u \phi \rangle \\ &= -\langle \nabla_h \cdot (uD)\phi \rangle + \langle\!\langle [\![Du]\!], \{\phi\} \rangle\!\rangle_\Gamma \\ &= \langle u \cdot \nabla_h \phi, D \rangle + \int_\Gamma u \cdot \left(\frac{1}{2}(D^+ n^+ + D^- n^-)(\phi^+ + \phi^-) \right. \\ &\qquad \left. - n^+ D^+ \phi^+ - n^- D^- \phi^- \right) \mathrm{d}S \end{aligned}$$

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$$= \langle u \cdot \nabla_h \phi, D \rangle + \int_\Gamma u \cdot \left(\frac{1}{2}(-D^+ n^+ \phi^+ + D^+ n^+ \phi^- + D^- n^- \phi^+ - D^- n^- \phi^-) \right) \mathrm{d}S$$

$$= \langle u \cdot \nabla_h \phi, D \rangle + \int_\Gamma u \cdot \left(\frac{1}{2}(-D^+ n^+ \phi^+ - D^+ n^- \phi^- - D^- n^+ \phi^+ - D^- n^- \phi^-) \right) \mathrm{d}S$$

$$= \langle u \cdot \nabla_h \phi, D \rangle - \langle\!\langle [\![u\phi]\!], \{D\} \rangle\!\rangle_\Gamma, \tag{6.53}$$

which is the standard discontinuous Galerkin centred flux scheme for the continuity equation for advected densities.

Similarly, by considering $\delta \langle D, f \rangle = 0$, we obtain

$$\delta D - Y^* D = 0, \tag{6.54}$$

where Y is such that $\delta \hat{\chi} + Y \hat{\chi} = 0$.

We can again use the overbar map to build Lagrangians with advected quantities defined on the whole of $GL(V_h^s, V_h^s)$. For example, the shallow water equations (with flat topography) have the (reduced) Lagrangian

$$\ell = \int_\Omega D \frac{|u|^2}{2} - \frac{gD^2}{2} \, \mathrm{d}x. \tag{6.55}$$

The discrete Lagrangian can then be written as

$$L\left(\frac{\partial}{\partial t} \hat{\chi}, \hat{\chi} \right) = \int_\Omega (\hat{\chi}^* D_0) \frac{\overline{|(\partial/\partial t)\hat{\chi} \circ \hat{\chi}^{-1}|^2}}{2} - \frac{g(\hat{\chi}^* D_0)^2}{2} \, \mathrm{d}x. \tag{6.56}$$

This has discrete reduced Lagrangian

$$\ell_h[D, X] = \int_\Omega D \frac{|\overline{X}|^2}{2} - \frac{gD^2}{2} \, \mathrm{d}x. \tag{6.57}$$

The reduced Hamilton's principle with non-holonomic constraints becomes

$$\delta \int_0^T \ell_h(X, D) \, \mathrm{d}t = 0, \tag{6.58}$$

with variations

$$\delta X = \frac{\partial}{\partial t} Y + [X, Y], \quad \delta D = Y^*, \tag{6.59}$$

and constraints $X = X_u$ for some $u \in W_h^r$, and $Y = Y_w$ for all $w \in W_h^r$.

This gives the equation

$$\left\langle \frac{\mathrm{d}}{\mathrm{d}t} \frac{\delta l}{\delta X_u}, X_w \right\rangle - \left\langle \frac{\delta l}{\delta X_u}, [X, X_w] \right\rangle + \left\langle \frac{\delta l}{\delta X_u}, X_w^* D \right\rangle \quad \text{for all } w \in W_h^r, \tag{6.60}$$

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which can be written as

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\delta l}{\delta X_u} + \mathrm{ad}^*_{X_u}\frac{\delta l}{\delta X_u} - \frac{\delta l}{\delta D}\diamond D \in (S^r_h)^*, \tag{6.61}$$

where

$$\left\langle \mathrm{ad}^*_X Y, Z\right\rangle = -\langle Y, [X,Z]\rangle,\ -\langle X\diamond Y, Z\rangle = \langle X, Y^* Z\rangle, \tag{6.62}$$

and $(S^r_h)^*$ is the dual space to S^r_h in $\mathfrak{gl}(V_h)$. This is the discrete analogue of (6.47).

6.6. *Compatible finite element variational discretizations: discrete conservation laws*

The goal of variational discretizations is to derive numerical methods that provide discrete analogues of conservation laws of the unapproximated equations. Noether's theorem can still be applied to non-holonomic variational principles without change, provided that the constraints are invariant under the relevant symmetry as well as the Lagrangian. The discrete variational principles discussed here are invariant under time translation, leading to the conservation of energy as usual. This is straightforward to check directly in the incompressible case of Natale and Cotter (2018) since the energy is

$$E = \langle \bar{A}_h, \bar{A}_h\rangle, \tag{6.63}$$

so the energy equation is obtained in (6.37) by taking $\bar{B}_h = \bar{A}_h$ and using antisymmetry of the bracket.

Regarding Kelvin's circulation theorem, Natale and Cotter (2018) demonstrated the same 'echo' in (6.17) for the compatible finite element case, which also emerges from Gawlik and Gay-Balmaz (2021*b*) in the case where the Lagrangian depends only on velocity and density, as expected. In the incompressible case, the conservation law takes the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle u, \overline{\hat{\chi} X_c \hat{\chi}^{-1}}\right\rangle = 0, \tag{6.64}$$

for all time-independent $c \in \mathring{W}^r_h$.

Gawlik and Gay-Balmaz (2021*b*) further extended the framework by introducing advected tracers (which can represent potential temperature, and salinity in the ocean), which are discretized as elements θ of V_h that can be acted on by velocity via $X_u\theta$ as above. This unlocks the variational discretization of all of the main variational models of geophysical fluid dynamics. The framework was further extended in Gawlik and Gay-Balmaz (2021*a*) to accommodate advected transported fluxes represented in W^r_h, leading to variational discretizations of magnetohydrodynamics.

6.7. *Variational time integrators*

So far in the this section we have only discussed the variational discretization in space, leading to a system that is still continuous in time. As set out in the original

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vision of Pavlov *et al.* (2011), the idea is to also discretize Hamilton's principle in time. Variational integrators arising from time discretization in Hamilton's principle have a long history, with the programme being formally set out in Marsden and West (2001). Variational time integration using a finite difference discretization in time was investigated in Gawlik and Gay-Balmaz (2021*b*). Since the kinetic energy is a nonlinear function of both the coordinate in V_h and its rate of change, any variational integrator will result in a system that requires the solution of an implicit nonlinear system (using Newton's method, for example). This contrasts with the case of classical mechanics, where the Lagrangian $L(z,(\partial/\partial t)z)$ splits into a kinetic energy depending only on $(\partial/\partial t)z$ and a potential energy depending only on z. This split makes explicit variational integrators possible in that case. Following Pavlov *et al.* (2011), Gawlik and Gay-Balmaz (2021*b*) made the choice of replacing $A(t) = (\partial/\partial t)\hat{\chi}\hat{\chi}^{-1}$ with $A_k = \tau^{-1}(\hat{\chi}_{k+1}\hat{\chi}_k^{-1})/\Delta t$, where $\tau\colon \mathfrak{gl}(V_h) \to G(V_h)$ is the Cayley transform

$$\tau(A) = \left(I - \frac{A}{2}\right)^{-1}\left(I + \frac{A}{2}\right), \tag{6.65}$$

with other possibilities for τ being discussed in Bou-Rabee and Marsden (2009). After this replacement, the variational integrator is derived by finding the stationary point of the resulting discrete action principle depending on $\hat{\chi}_{k+1}$ and $\hat{\chi}_k$. It was found through numerical experiments that the resulting scheme is only conditionally stable, requiring the condition $\delta t < Ch$. This is disappointing given that intensive computation is required to advance the solution by a small step. The nature of this stepsize requirement is an open problem in the area, as is the question of whether a variational integrator can be found that allows larger time-steps. Natale and Cotter (2018) used the implicit midpoint rule to discretize the semi-discrete variational discretization. The implicit midpoint rule is not known to be a variational integrator for such systems, but does have the property that it preserves any quadratic invariants of the time-continuous system, which includes the energy in the incompressible case.

7. Almost-Poisson brackets

An alternative, but related, route to structure preserving discretizations is found via Poisson bracket formulations.

Poisson brackets are bilinear skew-symmetric maps that take pairs of functionals on some space where the solutions of the PDE reside, which also satisfy the Jacobi identity,

$$\{A,\{B,C\}\} + \{B,\{C,A\}\} + \{C,\{A,B\}\} = 0, \tag{7.1}$$

for all functionals A, B, C. In the process of discretization of Poisson brackets for fluid dynamics, the Jacobi identity is lost, for similar reasons that the non-holonomic constraints are required for the variational discretizations of Section 6. Poisson brackets without the Jacobi identity are called 'almost-Poisson brackets',

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but we shall just use the term Poisson bracket in the rest of this article for brevity. Poisson brackets can have special functionals called Casimirs, which make the Poisson bracket vanish, that is, C is a Casimir if $\{F, C\} = 0$ for all functionals F. Then Casimirs are conserved by the dynamics since

$$\frac{\partial}{\partial t} C = -\{C, H\} = 0. \tag{7.2}$$

The goal of building discretizations using Poisson brackets is that they automatically conserve the Hamiltonian, and if any Casimirs survive the discretization process then they will be conserved as well. We shall discuss specific examples later.

The aim of building structure preserving discretizations for fluid PDEs using Poisson brackets was introduced in Morrison (1982) and Salmon (1983), although in fact the energy–enstrophy preserving discretizations in Arakawa (1966) are the first instance of a Poisson bracket discretization (but not presented that way), which was extended to the rotating shallow water equations and beyond in subsequent work by Arakawa, Sadourny and others (Sadourny, Arakawa and Mintz 1968, Sadourny 1972, 1975, Arakawa and Lamb 1977, 1981, Arakawa and Hsu 1990).

In the 2000s, when attention was focused much more on triangular and polygonal grids to provide a more uniform coverage of the sphere, the idea of using Poisson brackets was revived to produce energy conserving schemes (or to at least guide the design of practical schemes that are as energy-consistent as possible). This took place in a number of groups (Ringler, Thuburn, Klemp and Skamarock 2010, Skamarock *et al.* 2012, Eldred and Randall 2017, Gassmann and Herzog 2008, Gassmann 2013, Tort, Dubos and Melvin 2015, Dubos *et al.* 2015). There was also work on extending Poisson brackets to Nambu brackets in pursuit of additional conserved quantities in the method (Sommer and Névir 2009).

There have also been some interesting studies about the relevance of conservation for geophysical models. Dubinkina and Frank (2007) demonstrated the benefits of using energy–enstrophy conserving schemes to obtain correct statistical equilibria, and Thuburn, Kent and Wood (2014*b*) demonstrated that energy conservation is important to obtain realistic backscatter in under-resolved simulations of two-dimensional turbulence (provided that enstrophy is dissipated at the small scale). Dubinkina (2018) demonstrated that conserving both energy and enstrophy is important in the context of data assimilation. Even when structure preserving discretizations lead to systems of equations that are challenging to solve efficiently, it is useful to consider how they relate to more standard discretizations to see where conservation errors are being committed, and to see when they are likely to be large or small.

In this section we describe how Poisson brackets can be used to construct energy (and enstrophy) conserving schemes. This work has been heavily informed by previous works using finite difference methods, such as those cited above. We shall start by briefly discussing the two-dimensional incompressible Euler equations, the rotating shallow water equations and then vertical slice and three-dimensional

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models. We initially assume that we are solving the equations on a closed manifold (the surface of the sphere, or periodic boundary conditions, for example), and will return to the treatment of boundary conditions later.

7.1. Incompressible Euler equations: continuous theory

Returning to Arnold's variational formulation for incompressible flow in (6.9), we can reformulate as

$$\left\langle \frac{\partial m}{\partial t}, v \right\rangle + \left\langle \left[\frac{\delta H}{\delta m}, v \right], m \right\rangle = 0 \quad \text{for all } v \in \mathfrak{X}_{\text{vol}}(\Omega), \tag{7.3}$$

where

$$H(m) = \langle m, u \rangle - \ell(u), \tag{7.4}$$

and we take $m = \delta l / \delta u \in \mathfrak{X}_{\text{vol}}(\Omega)$, now inverting the relationship so that u is considered as an operator applied to m. Here we use the variational derivative $\delta F / \delta u \in \mathfrak{X}_{\text{vol}}(\Omega)$ defined by

$$\left\langle \frac{\delta F}{\delta u}, v \right\rangle = \lim_{\epsilon \to 0} \frac{1}{\epsilon} (F[u + \epsilon v] - F[u]). \tag{7.5}$$

Equation (7.3) is equivalent to the Poisson formulation

$$\frac{\partial}{\partial t} F[m] + \{F, H\} = 0, \tag{7.6}$$

for arbitrary functionals $F : \mathfrak{X}_{\text{vol}}(\Omega) \to \mathbb{R}$, with Poisson bracket

$$\{F, G\} = \int_\Omega \left[\frac{\delta G}{\delta m}, \frac{\delta F}{\delta m} \right] \cdot m \, \mathrm{d}x. \tag{7.7}$$

Since the Poisson bracket is antisymmetric, this leads immediately to conservation of the Hamiltonian,

$$\frac{\mathrm{d}}{\mathrm{d}t} H = -\{H, H\} + \frac{\partial H}{\partial t} = 0, \tag{7.8}$$

provided that H has no explicit dependence on time t.

For the two-dimensional incompressible Euler equations, a clear path towards deriving enstrophy conservation requires modification of the bracket (7.7) by changing variables $m \to u$. This produces the equivalent Poisson formulation

$$\frac{\partial}{\partial t} F[u] + \{F, H\}[u] = 0, \tag{7.9}$$

for all functionals $F : \mathfrak{X}_{\text{vol}}(\Omega) \to \mathbb{R}$, where

$$\{F, G\} = \int_\Omega \omega \left(\frac{\delta F}{\delta u} \right) \cdot \frac{\delta G}{\delta u}^{\perp} \, \mathrm{d}x, \tag{7.10}$$

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$\omega = \nabla^\perp \cdot u$, and

$$H = \frac{1}{2}\int_\Omega |u|^2 \,\mathrm{d}x. \tag{7.11}$$

The derivation of this bracket formulation from (7.7) is discussed in Morrison (1982) and Marsden and Weinstein (1983). Here, we just directly demonstrate that it leads to the incompressible Euler equations by computation. First, we compute $\delta H/\delta u = u$. For a linear functional $F[u] = \langle u, w\rangle$ with $w \in \mathfrak{X}_{\mathrm{vol}}(\Omega)$, (7.9) becomes

$$\langle u_t, w\rangle + \langle \omega, w \cdot u^\perp\rangle = 0 \quad \text{for all } w \in \mathfrak{X}_{\mathrm{vol}}(\Omega), \tag{7.12}$$

which is a weak formulation of the equation

$$u_t + \omega u^\perp + \nabla P = 0, \tag{7.13}$$

where P is some potential chosen so that $u_t \in \mathfrak{X}_{\mathrm{vol}}(\Omega)$ (because we only test against functions from $\mathfrak{X}_{\mathrm{vol}}(\Omega)$ in (7.13), so the equation is projected into $\mathfrak{X}_{\mathrm{vol}}(\Omega)$). Writing $P = \frac{1}{2}|u|^2 + p$, we obtain

$$u_t + u^\perp \nabla^\perp \cdot u + \nabla\frac{1}{2}|u|^2 + \nabla p = 0, \tag{7.14}$$

which becomes recognizable as the incompressible Euler equations after recalling the identity

$$(u \cdot \nabla)u = \omega u^\perp + \frac{1}{2}\nabla|u|^2. \tag{7.15}$$

Returning to the Poisson bracket (7.10), we find that it has an infinite number of Casimirs of the form

$$C_n[u] = \int_\Omega \omega^n \,\mathrm{d}x, \quad n = 1, 2, \ldots \tag{7.16}$$

To verify that C_n is a Casimir, we compute

$$\begin{aligned}\left\langle \frac{\delta C_n}{\delta u}, v\right\rangle &= n\int_\Omega \omega^{n-1}\nabla^\perp v \,\mathrm{d}x \quad \text{for all } v \in \mathfrak{X}_{\mathrm{vol}}(\Omega)\\ &= \int_\Omega \nabla^\perp(-n\omega^{n-1}) \cdot v \,\mathrm{d}x,\end{aligned} \tag{7.17}$$

having integrated by parts (we assume for now that there are now boundaries and so may ignore the surface term). Hence we conclude formally that

$$\frac{\delta C_n}{\delta u} = -n\nabla^\perp \omega^{n-1}. \tag{7.18}$$

Inserting into the Poisson bracket then gives

$$\begin{aligned}\{F, C_n\} &= -n\int_\Omega \omega \frac{\delta F}{\delta u} \cdot (\nabla^\perp \omega^{n-1})^\perp \,\mathrm{d}x\\ &= n\int_\Omega \omega \frac{\delta F}{\delta u} \cdot \nabla\omega^{n-1} \,\mathrm{d}x\end{aligned}$$

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$$= (n-1)\int_\Omega \frac{\delta F}{\delta u}\cdot\nabla\omega^n\,\mathrm{d}x$$
$$= -(n-1)\int_\Omega \omega^n \underbrace{\nabla\cdot\frac{\delta F}{\delta u}}_{=0}\,\mathrm{d}x = 0, \tag{7.19}$$

having integrated by parts again, for any functional F on $\mathfrak{X}_{\mathrm{vol}}(\Omega)$. We have

$$\nabla\cdot\frac{\delta F}{\delta u} = 0 \tag{7.20}$$

since

$$\frac{\delta F}{\delta u} \in \mathfrak{X}_{\mathrm{vol}}(\Omega). \tag{7.21}$$

Hence C_n is a conserved quantity for the Poisson dynamics from any Hamiltonian. In particular, C_1 is the *total vorticity*, whilst C_2 is the *enstrophy*, both of which provide strong constraints on two-dimensional incompressible turbulence.

7.2. Incompressible Euler equations: compatible finite element discretization

To make our compatible finite element discretization, we restrict u and w to the divergence-free subspace ζ_h of some chosen $H(\mathrm{div})$ finite element space $\mathbb{V}^1_h$ (such as Raviart–Thomas or Brezzi–Douglas–Marini on triangles). We have to make a further approximation since $\nabla^\perp\cdot u$ is not defined for $H(\mathrm{div})$ spaces, and so we define $\omega_h \in \mathbb{V}^0_h$, such that

$$\langle\gamma,\omega_h\rangle = -\langle\nabla^\perp\gamma,u\rangle \quad \text{for all } \gamma\in\mathbb{V}^0_h, \tag{7.22}$$

that is, ω_h is defined from the approximated weak curl of u, the dual of the $\nabla^\perp$ operator restricted to $\mathbb{V}^0_h$ and $\mathbb{V}^1_h$. Note that this is where we have used the absence of boundary, otherwise there would be a boundary term causing complications that we shall discuss later. Having defined ω_h, we write the discrete Poisson bracket as

$$\{F,G\} = \int_\Omega \omega_h \frac{\delta F}{\delta u}\cdot\frac{\delta G}{\delta u}^{\perp}\,\mathrm{d}x, \tag{7.23}$$

where F and G are now functionals on $\mathbb{V}^1_h$. With the same Hamiltonian (7.11) now restricted to $\mathbb{V}^1_h$, the Poisson formulation implies the following dynamics for $u\in\zeta_h$:

$$\langle w,u_t\rangle + \langle\omega_h w\cdot u^\perp\rangle = 0 \quad \text{for all } w\in\zeta_h. \tag{7.24}$$

The discrete Hamiltonian is conserved as usual through the antisymmetry of the bracket and the time-independence of H. Concerning Casimirs of the bracket, we can repeat the earlier calculation for functionals C_n computed with ω_h substituted for ω, that is,

$$C_{n,h}[u] = \int_\Omega \omega_h^n\,\mathrm{d}x. \tag{7.25}$$

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Following (7.17), we obtain

$$\left\langle \frac{\delta C_{n,h}}{\delta v} \right\rangle = \int_\Omega \nabla^\perp(-n\omega^{n-1}) \cdot v \, \mathrm{d}x \quad \text{for all } v \in \zeta_h, \tag{7.26}$$

but now can only conclude that

$$\frac{\delta C_{n,h}}{\delta v} = P_1\left(-n\nabla^\perp \omega^{n-1}\right), \tag{7.27}$$

where P_1 is the L^2 projection into ζ_h, which prevents us from showing that $C_{n,h}$ is a Casimir for $n > 2$. However, when $n = 1$, we obtain that $\delta C_{1,h}/\delta v = 0$ (so $C_{1,h}$ is trivially conserved, just as C_1 is for the unapproximated case). When $n = 2$, we have $\nabla^\perp \omega \in \mathbb{V}_h^1$ by the embedding property of the discrete de Rham complex, and then a calculation identical to (7.19) shows that $\{C_{2,h}, G\} = 0$ for any functional G on ζ_h, and hence the numerical enstrophy $C_{2,h}$ is a Casimir and is conserved for dynamics generated from any Hamiltonian. Hence this scheme conserves energy, total vorticity, and enstrophy.

To make a practical implementation of the scheme, one can follow two approaches. The main hurdle is that the scheme is defined on ζ_h, and not the whole of $\mathbb{V}_h^1$. Since $\nabla\cdot$ maps from $\mathbb{V}_h^1$ onto $\mathbb{V}_h^2$, the divergence-free subspace ζ_h is equivalently represented as

$$\zeta_h = \left\{ u \in \mathbb{V}_h^1 : \int_\Omega \phi \nabla \cdot u \, \mathrm{d}x = 0 \ \text{ for all } \phi \in \mathbb{V}_h^2 \right\}. \tag{7.28}$$

Hence we can equivalently write the following system for $(\omega, u, P) \in \mathbb{V}_h^0 \times \mathbb{V}_h^1 \times \mathbb{V}_h^2$ such that

$$\langle \gamma, \omega \rangle - \langle \nabla^\perp \gamma, u \rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}_h^0, \tag{7.29}$$

$$\langle w, u_t \rangle + \langle w, \omega u^\perp \rangle - \langle \nabla \cdot w, P \rangle = 0 \quad \text{for all } w \in \mathbb{V}_h^1, \tag{7.30}$$

$$\langle \phi, \nabla \cdot u \rangle = 0 \quad \text{for all } \phi \in \mathbb{V}_h^2. \tag{7.31}$$

It can easily be checked that the solution satisfies $\nabla \cdot u = 0$ in L^2. Selecting $w \in \zeta_h \subset \mathbb{V}_h^1$ makes the P term disappear and we recover (7.24). This formulation builds a bridge to the shallow water and compressible systems that we shall look at later.

On the other hand, for $u \in \zeta_h$ we can directly parametrize $u = \nabla^\perp \psi$ for $\psi \in \mathbb{V}_h^0$ and choose $w = \nabla^\perp \beta$ in (7.24) for all $\beta \in \mathbb{V}_h^0$, and we obtain

$$\langle \gamma, \omega \rangle + \langle \nabla \gamma, \nabla \psi \rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}_h^0, \tag{7.32}$$

$$\langle \nabla \beta, \nabla \psi_t \rangle + \langle \nabla \beta, \omega \nabla^\perp \psi \rangle = 0 \quad \text{for all } \beta \in \mathbb{V}_h^0, \tag{7.33}$$

which is a discretization of the incompressible Euler equation in vorticity–stream-function form,

$$\omega_t + \nabla \cdot (\omega \nabla^\perp \psi) = 0, \quad -\nabla^2 \psi = \omega. \tag{7.34}$$

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This formulation was presented in Liu and E (2001), where it was analysed in the viscous case, but the energy conservation of the inviscid equations did form an important part of the proof. A related scheme was presented in Liu and Shu (2000), but with the vorticity in a discontinuous space, with appropriate jump terms defining the fluxes between cells. With an average flux, the energy and enstrophy are both conserved. If a Lax–Friedrichs flux is used, then energy is still conserved but enstrophy is dissipated (as is appropriate for long-time simulations of cascading two-dimensional vortex dynamics). It is possible to modify the Poisson bracket so that enstrophy is dissipated in this way, with the antisymmetric formulation still conserving energy, as we shall see later. Liu and Shu (2000) proved convergence for both types of fluxes. This formulation and analysis was extended by Bernsen, Bokhove and van der Vegt (2006) to the quasigeostrophic model of large-scale rotating geophysical fluid dynamics, including the case with islands in the flow (considering the fluid as an ocean).

To extend the conservation properties to a fully discrete method, one can use the implicit midpoint rule, which conserves all quadratic invariants of the continuous-time system. This includes energy and enstrophy (or just energy where enstrophy is dissipated) in the incompressible Euler case.

7.3. Rotating shallow water equations: continuous theory

Moving on to the rotating shallow water equations, it is tempting to continue working with the vorticity–streamfunction formulation above. However, this places a limitation on the possibilities of extension to three-dimensional models, complicates the boundary conditions, and is not preferred by practitioners since the prognostic variables are not quantities that are directly measurable. Hence we must address the challenge of finding a compatible finite element discretization of the rotating shallow water equations using velocity u and layer depth D.

We start from the Lie–Poisson formulation of the rotating shallow water equations given by

$$H = \int_\Omega \frac{1}{2D}|m|^2 + gD\left(\frac{D}{2} + b\right) \mathrm{d}x, \tag{7.35}$$

$$\{F, G\} = \left\langle \left[\frac{\delta G}{\delta m}, \frac{\delta F}{\delta m}\right], m\right\rangle + \left\langle \frac{\delta F}{\delta D}, \nabla\cdot\left(D\frac{\delta G}{\delta m}\right)\right\rangle - \left\langle \frac{\delta G}{\delta D}, \nabla\cdot\left(D\frac{\delta F}{\delta m}\right)\right\rangle, \tag{7.36}$$

where m is defined by

$$\int_\Omega m\cdot v\,\mathrm{d}x = \int_\Omega D(u+R)\cdot v\,\mathrm{d}x \quad \text{for all } v\in\mathfrak{X}(\Omega), \tag{7.37}$$

where $\nabla^\perp\cdot R = f$, the Coriolis parameter. These equations emerge from the reduced Hamilton's principle with advected density D after applying the Legendre transform as described in Holm *et al.* (1998). Following the incompressible case, if we want enstrophy conservation to emerge then we need to change variables to

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(u, D); this leads to the equivalent Poisson bracket formulation

$$H = \frac{1}{2}\int_\Omega D\|u\|^2 + gD\left(\frac{D}{2} + b\right)\mathrm{d}x, \tag{7.38}$$

$$\{F, G\} = \left\langle q, \frac{\delta F}{\delta u}\cdot\frac{\delta G}{\delta u}^\perp\right\rangle - \left\langle \nabla\cdot\frac{\delta F}{\delta u}, \frac{\delta G}{\delta D}\right\rangle + \left\langle \nabla\cdot\frac{\delta G}{\delta u}, \frac{\delta F}{\delta D}\right\rangle, \tag{7.39}$$

where $q = (\nabla^\perp\cdot u + f)/D$ is the potential vorticity. After computing the variational derivatives

$$\frac{\delta H}{\delta u} = Du, \tag{7.40}$$

$$\frac{\delta H}{\delta D} = \frac{1}{2}\|u\|^2 + g(D + b), \tag{7.41}$$

and substituting into the Poisson bracket equation $F_t + \{F, H\}$, we formally obtain

$$u_t + qDu^\perp + \nabla\left(\frac{1}{2}|u|^2 + g(D + b)\right) = 0, \tag{7.42}$$

$$D_t + \nabla\cdot(uD) = 0, \tag{7.43}$$

which we recognize as the rotating shallow water equations in vector-invariant form. We define functionals C_n (which will turn out to be Casimirs) by

$$C_n[u, D] = \int_\Omega Dq^n\,\mathrm{d}x. \tag{7.44}$$

To compute the variational derivatives, given $\epsilon > 0$ and $(v, \phi) \in H(\mathrm{div}) \times L^2$, writing $D_\epsilon = D + \epsilon\phi$, $u_\epsilon = u + \epsilon v$, we define $q_\epsilon \in H^1$ such that

$$\langle\gamma, D_\epsilon q_\epsilon\rangle = -\langle\nabla^\perp\gamma, u_\epsilon\rangle + \langle\gamma, f\rangle \quad \text{for all } \gamma \in H^1, \tag{7.45}$$

noting that $q_\epsilon|_{\epsilon=0} = q$ (after integrating by parts and using the lack of surface term in a domain without boundary). Then

$$\begin{aligned}
\left\langle\frac{\delta C_n}{\delta v}, v\right\rangle + \left\langle\frac{\delta C_n}{\delta D}, \phi\right\rangle &= \lim_{\epsilon\to 0}\frac{1}{\epsilon}(C_n[u + \epsilon v, D + \epsilon\phi] - C_n[u, D]) \\
&= \int_\Omega \lim_{\epsilon\to 0}\frac{D_\epsilon q_\epsilon^n - Dq^n}{\epsilon}\,\mathrm{d}x \\
&= \int_\Omega \frac{\mathrm{d}}{\mathrm{d}\epsilon}\Big|_{\epsilon=0} D_\epsilon q_\epsilon^n\,\mathrm{d}x \\
&= \left\langle q_\epsilon^{n-1}\Big|_{\epsilon=0}, \frac{\mathrm{d}}{\mathrm{d}\epsilon}\Big|_{\epsilon=0} D_\epsilon q_\epsilon\right\rangle \\
&\quad + \left\langle (n-1)q_\epsilon^{n-2}\Big|_{\epsilon=0}\frac{\mathrm{d}}{\mathrm{d}\epsilon}\Big|_{\epsilon=0} q_\epsilon, D_\epsilon q_\epsilon\right\rangle
\end{aligned}$$

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$$= n\left\langle q_\epsilon^{n-1}\Big|_{\epsilon=0}, \frac{\mathrm{d}}{\mathrm{d}\epsilon}\Big|_{\epsilon=0} D_\epsilon q_\epsilon \right\rangle - \left\langle (n-1) q_\epsilon^n\Big|_{\epsilon=0}, \frac{\mathrm{d}}{\mathrm{d}\epsilon}\Big|_{\epsilon=0} D_\epsilon \right\rangle, \tag{7.46}$$

From (7.45) we have

$$\left\langle \gamma, \frac{\mathrm{d}}{\mathrm{d}\epsilon}\Big|_{\epsilon=0} D_\epsilon q_\epsilon \right\rangle = -\langle \nabla^\perp \gamma, v\rangle \quad \text{for all } \gamma \in H^1 \tag{7.47}$$

(correcting a typographic error in equation 58 of McRae and Cotter (2014)), and hence we have

$$\left\langle \frac{\delta C_n}{\delta v}, v \right\rangle + \left\langle \frac{\delta C_n}{\delta D}, \phi \right\rangle = n\langle \nabla^\perp q^{n-1}, v\rangle - \langle (n-1) q^n, \phi\rangle, \tag{7.48}$$

that is,

$$\frac{\delta C_n}{\delta v} = n\nabla^\perp q^{n-1}, \quad \frac{\delta C_n}{\delta D} = -(n-1) q^n. \tag{7.49}$$

Then, inserting into the Poisson bracket (7.39), we obtain

$$\begin{aligned} \{C_n, G\} &= \Bigg\langle \underbrace{nq\nabla^\perp q^{n-1}}_{=(n-1)\nabla^\perp q^n}, \frac{\delta G}{\delta u}^\perp \Bigg\rangle \\ &\quad - \Bigg\langle \underbrace{\nabla\cdot n\nabla^\perp q^{n-1}}_{=0}, \frac{\delta G}{\delta D}\Bigg\rangle + \left\langle (n-1) q^n, \nabla\cdot\frac{\delta G}{\delta u}\right\rangle \\ &= \left\langle (n-1)\nabla q^n, \frac{\delta G}{\delta u}\right\rangle - \left\langle (n-1) q^n, \nabla\cdot\frac{\delta G}{\delta u}\right\rangle = 0, \end{aligned} \tag{7.50}$$

where the last line is obtained by integrating by parts, and hence C_n is a Casimir of the bracket (7.39), and so it is a conserved quantity of the dynamics for any Hamiltonian. Another, more simple, Casimir is the mass

$$M[u, D] = \int_\Omega D \,\mathrm{d}x, \tag{7.51}$$

with variational derivatives

$$\frac{\delta M}{\delta u} = 0, \quad \frac{\delta M}{\delta D} = 1, \tag{7.52}$$

and hence

$$\{M, G\} = \left\langle \nabla\cdot\frac{\delta G}{\delta u}, 1\right\rangle = \int_\Omega \nabla\cdot\frac{\delta G}{\delta D}\,\mathrm{d}x = 0, \tag{7.53}$$

using the divergence theorem (assuming no boundary currently), so mass is also a Casimir of the bracket and is conserved for any Hamiltonian.

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7.4. *Rotating shallow water equations: Poisson bracket discretization*

To produce a discretization of this structure, McRae and Cotter (2014) simply took the structure (7.38)–(7.39), restricted (u, D) to $\mathbb{V}_h^1 \times \mathbb{V}_h^2$, and replaced q with the discrete approximation $q \in \mathbb{V}_h^0$, with

$$\langle \gamma, Dq \rangle = -\langle \nabla^\perp \gamma, u \rangle + \langle \gamma, f \rangle \quad \text{for all } \gamma \in \mathbb{V}_h^0, \tag{7.54}$$

following the exposition for the discretization for incompressible Euler equations above. Then we obtain

$$\left\langle w, \frac{\delta H}{\delta u} - Du \right\rangle = 0 \quad \text{for all } w \in \mathbb{V}_h^1, \tag{7.55}$$

$$\left\langle \phi, \frac{\delta H}{\delta D} - \frac{1}{2}|u|^2 - g(D+b) \right\rangle = 0 \quad \text{for all } \phi \in \mathbb{V}_h^2, \tag{7.56}$$

that is,

$$\frac{\delta H}{\delta u} = P_1(Du), \quad \frac{\delta H}{\delta D} = P_2\left(\frac{1}{2}|u|^2 + g(D+b)\right), \tag{7.57}$$

where P_1 and P_2 are the L^2 projections into $\mathbb{V}_h^1$ and $\mathbb{V}_h^2$, respectively. To derive the equations of motion, we take $F[u, D] = \langle w, u \rangle + \langle \phi, D \rangle$ for $w, \phi \in \mathbb{V}_h^1 \times \mathbb{V}_h^2$, so that

$$\frac{\delta F}{\delta u} = w, \quad \frac{\delta F}{\delta D} = \phi, \tag{7.58}$$

and substitute into the Poisson dynamics to obtain

$$\begin{aligned}
\langle w, u_t \rangle + \langle \phi, D_t \rangle &= \frac{\partial}{\partial t} F \\
&= -\{F, H\} \\
&= -\langle q, w \cdot P_1(Du)^\perp \rangle + \left\langle \nabla \cdot w, P_2\left(\frac{1}{2}|u|^2 + g(D+b)\right) \right\rangle \\
&\quad - \langle \nabla \cdot P_1(Du), \phi \rangle \\
&= -\langle q, w \cdot P_1(Du)^\perp \rangle + \left\langle \nabla \cdot w, \frac{1}{2}|u|^2 + gD \right\rangle - \langle \nabla \cdot P_1(Du), \phi \rangle
\end{aligned} \tag{7.59}$$

for all $w, \phi \in \mathbb{V}_h^1 \times \mathbb{V}_h^2$, where we were able to drop the P_2 since the result of the projection was in an L^2 inner product with $\nabla \cdot w \in P_2$ (so the discrete de Rham complex is crucial here). Writing $m = P_1(Du)$, we put everything together as

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$(u, D, q, m) \in \mathbb{V}_h^1 \times \mathbb{V}_h^2 \times \mathbb{V}_h^0 \times \mathbb{V}_h^1$, such that

$$\langle w, u_t \rangle + \langle qw, m^\perp \rangle - \left\langle \nabla \cdot w, \frac{1}{2}|u|^2 + g(D+b) \right\rangle = 0 \quad \text{for all } w \in \mathbb{V}_h^1, \tag{7.60}$$

$$\langle \phi, D_t + \nabla \cdot m \rangle = 0 \quad \text{for all } \phi \in \mathbb{V}_h^2, \tag{7.61}$$

$$\langle \gamma, qD \rangle + \langle \nabla^\perp \gamma, u \rangle - \langle \gamma, f \rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}_h^0, \tag{7.62}$$

$$\langle v, m - uD \rangle = 0 \quad \text{for all } v \in \mathbb{V}_h^1. \tag{7.63}$$

This is a set of coupled equations which must be solved together, but since equations (7.62)–(7.63) do not contain time derivatives, q and m may be reconstructed at any time from u and D. Since the equations are derived from a Poisson bracket formulation, we can immediately deduce that they conserve the Hamiltonian. Concerning the Casimirs, we make the same calculations for mass M as for the undiscretized case, obtaining

$$\frac{\delta M}{\delta u} = 0, \quad \frac{\delta M}{\delta D} = P_1(D) = 1. \tag{7.64}$$

For C_n, we can only make use of (7.45) when $n = 1$ (so that $\gamma = 1$) or $n = 2$ (so that $\gamma = q_\epsilon$), leading to

$$\frac{\delta C_n}{\delta u} = n(\nabla^\perp q^{n-1}), \quad \frac{\delta C_n}{\delta D} = -(n-1)P_2(q^n). \tag{7.65}$$

(7.50) then follows but only for $n = 1, 2$,

$$\begin{aligned} \{C_n, G\} &= \left\langle nq\nabla^\perp q^{n-1}, \frac{\delta G}{\delta u}^\perp \right\rangle \\ &\quad - \left\langle n \underbrace{\nabla \cdot \nabla^\perp q^{n-1}}_{=0}, \frac{\delta G}{\delta u} \right\rangle + \left\langle P_2((n-1)q^n), \nabla \cdot \frac{\delta G}{\delta u} \right\rangle \\ &= \left\langle nq\nabla^\perp q^{n-1}, \frac{\delta G}{\delta u}^\perp \right\rangle + \left\langle (n-1)q^n, \nabla \cdot \frac{\delta G}{\delta u} \right\rangle = 0, \end{aligned} \tag{7.66}$$

where we may integrate by parts since $\delta G/\delta u \in \mathbb{V}_h^1 \subset H(\text{div})$ and $q^n \in \mathbb{V}_h^0 \subset H^1$. Hence C_n is a Casimir for $n = 1$ (total vorticity) and $n = 2$ (enstrophy).

McRae and Cotter (2014) verified these conservation properties in numerical experiments, and showed second-order convergence with h for the scheme with the $BDFM_1$–DG_1 finite element spaces on triangles ($BDFM_1$ is a slightly more exotic variant which has an intermediate number of degrees of freedom between BDM_1 and RT_1, which results in a 2:1 ratio of velocity to pressure degrees of freedom).

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The Poisson bracket approach has been extended to other compatible spaces with various motivations. Eldred *et al.* (2019) used finite element spaces built around splines to form higher-order discrete de Rham complexes. These spaces have the same degrees of freedom as the lowest-order Q_1–RT_0–DG_0 complex on quadrilaterals, and achieve higher order by making use of degrees of freedom from a patch of neighbouring cells. The advantage is that this removes the jump in the dispersion relation for gravity waves in higher-order spaces on quadrilaterals, as discussed in Section 3.5. The price to be paid is that there is increased interelement coupling, and that there are some technicalities at the boundaries between patches of structured quadrilaterals, for example at the edges and vertices of the cube upon which a cubed sphere mesh is constructed. Since Hamiltonian and the Poisson brackets are the same, the only thing that has changed is the finite element spaces, which still satisfy the discrete de Rham complex, so energy–enstrophy conservation follows directly.

Lee *et al.* (2018) extended the method to mixed mimetic spectral elements, which are a variant of mixed elements using spectral element histopolation functions to construct high-order spaces. The usual spectral element technique of using incomplete quadrature then leads to diagonal mass matrices for the continuous space $\mathbb{V}_h^0$ without losing the discrete de Rham complex property. Again, since the Hamiltonian and Poisson brackets are the same (excepting some details on quadrature rules, where care must be taken), and the new finite element spaces still satisfy the discrete de Rham complex, the energy–enstrophy conservation follows directly. Lee and Palha (2018) extended these spaces to the surface of the sphere.

7.5. *Poisson integrators*

To extend these conservation properties to a fully discrete method after time discretization, we need to look beyond the implicit midpoint rule into the more general case of Poisson integrators. To make this generalization, we write the Poisson bracket as

$$\{F, G\} = A\left(\frac{\delta F}{\delta z}, \frac{\delta G}{\delta z}; z\right), \tag{7.67}$$

where $z \in W$ comprises the dynamic fields (i.e. $z = (u, D)$ and $W = \mathbb{V}_h^1 \times \mathbb{V}_h^2$ for the case of the shallow water equations). We use this notation to express that Poisson brackets are bilinear in $(\delta F/\delta z, \delta G/\delta z)$ but with possibly arbitrary additional dependence on z, which acts as a coefficient. When there is no explicit dependence on z, we obtain linear dynamics, and the z dependency encodes nonlinear dynamics. From the properties of the Poisson bracket, A is bilinear and antisymmetric in $\delta F/\delta z$ and $\delta G/\delta z$. To derive one particular Poisson integrator, we write $z(s) = z^n + s(z^n - z^{n+1})$, and seek z^{n+1} such that

$$\int_0^{\Delta t} \left(\frac{\partial}{\partial t} F[z(s)] + A\left(\frac{\delta F}{\delta z}[z(s)], \frac{\delta H}{\delta z}[z(s)]; z^{n+1/2}\right)\right) \beta(s)\, \mathrm{d}s = 0, \tag{7.68}$$

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for all linear functions $\beta(s)$. In other words, we replace the bracket $\{F, G\}$ by

$$\{F, G\} = A\left(\frac{\delta F}{\delta z}, \frac{\delta G}{\delta z}; z^{n+1/2}\right), \tag{7.69}$$

where $z^{n+1/2} = (z^n + z^{n+1})/2$, and project the equation onto linear dynamics in time. We observe energy conservation since taking $F = H$ and $\beta = 1$ leads to

$$\begin{aligned}\frac{H[z^{n+1}] - H[z^n]}{\Delta t} &= \int_0^{\Delta t} \frac{\partial}{\partial s} H[z(s)]\,\mathrm{d}s \\ &= -\int_0^{\Delta t} \underbrace{A\left(\frac{\delta H}{\delta z}[z(s)], \frac{\delta H}{\delta z}[z(s)]; z^{n+1/2}\right)}_{=0}\,\mathrm{d}s = 0,\end{aligned} \tag{7.70}$$

by antisymmetry.

This formulation leads to a practical method since taking $F[z] = \langle w, z\rangle$ for $w \in W$ and $\beta = 1$ gives

$$\left\langle w, z^{n+1} - z^n\right\rangle + A\left(w, \int_0^{\Delta t} \frac{\delta H}{\delta z}[z(s)]\,\mathrm{d}s; z^{n+1/2}\right) = 0, \tag{7.71}$$

by linearity in the second argument. This scheme was introduced along with higher-order variants as a larger set of Poisson integrators in Hairer (2010) and Cohen and Hairer (2011). The easiest way to obtain implementable formulae for the scheme is to choose a quadrature rule for the time integral in (7.71) such that the integral is exact. This is possible whenever the Hamiltonian is polynomial. For example, when the Hamiltonian is quadratic, $\delta H/\delta z$ is linear, and the midpoint rule

$$\int_0^{\Delta t} \frac{\delta H}{\delta z}[z(s)]\,\mathrm{d}s = \frac{1}{2}\left(\frac{\delta H}{\delta z}\left[z^n + \frac{1}{2}\left(z^{n+1} - z^n\right)\right]\right) \tag{7.72}$$

(evaluated at $s = 1/2$ with weight 1) is exact; the scheme is then equivalent to the implicit midpoint rule.

For the rotating shallow water equation scheme described above, the Hamiltonian is cubic, so a two-point quadrature must be used to compute the time integral involving the quadratic derivatives of the Hamiltonian exactly. We obtain the scheme

$$\begin{aligned}\left\langle w, u^{n+1}\right\rangle + \left\langle \phi, D^{n+1}\right\rangle = \langle w, u^n\rangle + \langle \phi, D^n\rangle \\ - \Delta t A\left((w, \phi), \left(\overline{\frac{\delta H}{\delta u}}, \overline{\frac{\delta H}{\delta D}}\right); \left(u^{n+1/2}, D^{n+1/2}\right)\right)\end{aligned} \tag{7.73}$$

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for all $(w, \phi) \in \mathbb{V}_h^1 \times \mathbb{V}_h^2$, where

$$\begin{aligned}\overline{\frac{\delta H}{\delta u}} &= P_1\left[m^{n+1/2}\right] \\ &= P_1\frac{1}{3}\left(D^n u^n + \frac{1}{2}D^n u^{n+1} + \frac{1}{2}D^{n+1}u^n + D^{n+1}u^{n+1}\right), \qquad (7.74)\\ \overline{\frac{\delta H}{\delta D}} &= P_2\left(\pi^{n+1/2}\right) \\ &= P_2\left(\frac{1}{6}\left(|u^n|^2 + u^n\cdot u^{n+1} + |u^{n+1}|^2\right) + \frac{g}{2}\left(D^{n+1}+D^n\right) + b\right). \qquad (7.75)\end{aligned}$$

This can be implemented as

$$\left(u^{n+1}, D^{n+1}, q^{n+1/2}, \overline{m}^{n+1/2}\right) \in \mathbb{V}_h^1 \times \mathbb{V}_h^2 \times \mathbb{V}_h^0 \times \mathbb{V}_h^1 \qquad (7.76)$$

such that

$$\begin{aligned}\left\langle w, u^{n+1}-u^n\right\rangle + \Delta t\left\langle w, q^{n+1/2}\left(\overline{m}^{n+1/2}\right)^\perp\right\rangle & \\ -\Delta t\left\langle \nabla\cdot w, \pi^{n+1/2}\right\rangle = 0 \quad \text{for all } w \in \mathbb{V}_h^1, & \qquad (7.77)\\ \left\langle \phi, D^{n+1}-D^n\right\rangle + \Delta t\left\langle \phi, \nabla\cdot\overline{m}^{n+1/2}\right\rangle = 0 \quad \text{for all } \phi \in \mathbb{V}_h^2, & \qquad (7.78)\\ \left\langle \gamma, D^{n+1/2}q^{n+1/2}\right\rangle + \left\langle \nabla^\perp\gamma, u^{n+1/2}\right\rangle - \left\langle \gamma, f\right\rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}_h^0, & \qquad (7.79)\\ \left\langle v, \overline{m}^{n+1/2} - m^{n+1/2}\right\rangle = 0 \quad \text{for all } v \in \mathbb{V}_h^1, & \qquad (7.80)\end{aligned}$$

with $m^{n+1/2}$, $\pi^{n+1/2}$ defined as above. This scheme is similar, but not identical, to the implicit midpoint rule, but results in energy conservation. Cohen and Hairer (2011) showed that this class of Poisson integrators also preserves Casimirs that are at most quadratic functions of the state space variables. This covers mass and total vorticity but not enstrophy, which is a non-polynomial function of u and D. Finding Poisson integrators that preserve enstrophy for this discrete formulation of the rotating shallow water equations is an open problem.

7.6. Enstrophy conservation on domains with boundaries

Something that we have neglected from our discussion so far is the case when the domain Ω has an exterior boundary. This is important when extending these tools to ocean applications (where there are coastlines). When boundaries are present, we consider the subcomplex

$$\begin{array}{ccccc} \mathring{H}^1 & \xrightarrow{\nabla^\perp} & \mathring{H}(\mathrm{div}) & \xrightarrow{\nabla\cdot} & L^2 \\ \downarrow{\scriptstyle \pi_0} & & \downarrow{\scriptstyle \pi_1} & & \downarrow{\scriptstyle \pi_2} \\ \mathring{\mathbb{V}}_h^0 & \xrightarrow{\nabla^\perp} & \mathring{\mathbb{V}}_h^1 & \xrightarrow{\nabla\cdot} & \mathbb{V}_h^2, \end{array} \qquad (7.81)$$

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where

$$\mathring{H}_1 = \{\phi \in H^1 : \ \mathrm{tr}_{\partial\Omega}\, \phi = 0\}, \tag{7.82}$$

$$\mathring{\mathbb{V}}^0_h = \left\{\phi \in \mathbb{V}^0_h : \ \mathrm{tr}_{\partial\Omega}\, \phi = 0\right\}, \tag{7.83}$$

$$\mathring{H}(\mathrm{div}) = \{u \in H(\mathrm{div}) : \ \mathrm{tr}_{\partial\Omega}\, u \cdot n = 0\}, \tag{7.84}$$

$$\mathring{\mathbb{V}}^1_h = \left\{u \in \mathbb{V}^1_h : \ \mathrm{tr}_{\partial\Omega}\, u \cdot n = 0\right\}, \tag{7.85}$$

and where tr is the boundary trace operator. When a boundary is present, we must modify (7.54) to incorporate a boundary integral,

$$\langle \gamma, Dq\rangle = -\langle \nabla^\perp \gamma, u\rangle + \langle\!\langle \gamma, n^\perp \cdot u\rangle\!\rangle + \langle \gamma, f\rangle \quad \text{for all } \gamma \in \mathbb{V}^0_h, \tag{7.86}$$

where $\langle\!\langle \cdot, \cdot \rangle\!\rangle$ is the usual L^2 inner product on $\partial\Omega$. This is necessary because q does not vanish on the boundary in general. One can then try to proceed using this modified definition of q in the Poisson bracket, now defined over $\mathring{\mathbb{V}}_1 \times \mathbb{V}^2_h$. The proof of enstrophy conservation then fails because although $\nabla^\perp q \in \mathbb{V}^1_h$, in general $\nabla^\perp q \notin \mathring{\mathbb{V}}_1$, because q is not constant on the boundary. One possible solution is to restrict $q \in \mathring{\mathbb{V}}^0_h$, and use (7.54) with test functions in $\mathring{\mathbb{V}}^0_h$, so that $\nabla^\perp q \in \mathring{\mathbb{V}}^1_h$. This recovers enstrophy conservation, but at the expense of consistency as it commits a first-order error in forcing q to be zero on the boundary.

An alternative solution presented in Bauer and Cotter (2018) is to split $\mathbb{V}^0_h = \mathring{\mathbb{V}}^0_h \oplus (\mathring{\mathbb{V}}^0_h)^\perp$, where $(\mathring{\mathbb{V}}^0_h)^\perp$ is the L^2-orthogonal complement of $\mathring{\mathbb{V}}^0_h$ in $\mathbb{V}^0_h$. We then extend the solution space to $(u, D, Z') \in \mathring{\mathbb{V}}^1_h \times \mathbb{V}^2_h \times (\mathring{\mathbb{V}}^0_h)^\perp$, and define the bracket

$$\begin{aligned}\{F, G\} = &\left\langle q, \frac{\delta F}{\delta u} \cdot \frac{\delta G}{\delta u}^\perp \right\rangle - \left\langle \nabla \cdot \frac{\delta F}{\delta u}, \frac{\delta G}{\delta D}\right\rangle + \left\langle \nabla \cdot \frac{\delta G}{\delta u}, \frac{\delta F}{\delta D}\right\rangle \\ &+ \left\langle \nabla \frac{\delta F}{\delta Z'}, q\frac{\delta G}{\delta u}\right\rangle - \left\langle \nabla \frac{\delta G}{\delta Z'}, q\frac{\delta F}{\delta u}\right\rangle,\end{aligned} \tag{7.87}$$

with the same Hamiltonian, where $q \in \mathbb{V}^0_h$ such that

$$\langle \gamma, qD\rangle - \langle \gamma, f + \mathring{Z} + Z'\rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}^0_h, \tag{7.88}$$

$$\langle \gamma, \mathring{Z}\rangle - \langle \nabla^\perp \gamma, u\rangle = 0 \quad \text{for all } \gamma \in \mathring{\mathbb{V}}^0_h. \tag{7.89}$$

Here, Z' represents the contribution to the vorticity from the boundary, which would normally be given by

$$\langle \gamma, Z'\rangle = -\langle \nabla^\perp \gamma, u\rangle + \langle\!\langle \gamma, n^\perp \cdot u\rangle\!\rangle + \langle \gamma, f\rangle \quad \text{for all } \gamma \in (\mathring{\mathbb{V}}^0_h)^\perp. \tag{7.90}$$

However, here we just ensure that Z' satisfies this condition initially, and that at future times Z' has its own dynamics consistent with the potential vorticity equation

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as we shall see later (and see Section 8 for further discussion of this). Since the Hamiltonian does not depend on Z', we have $\delta H/\delta u$ and $\delta H/\delta D$ as before, and $\delta H/\delta Z' = 0$. Thus the u_t and D_t equations are unchanged, and we have

$$\left\langle \gamma, Z_t' \right\rangle = \left\langle \nabla\gamma, q\frac{\delta H}{\delta u} \right\rangle = \langle \nabla\gamma, mq \rangle \quad \text{for all } \gamma \in (\mathring{\mathbb{V}}^0_h)^\perp. \tag{7.91}$$

The bracket is antisymmetric, so the Hamiltonian is conserved.

To check whether this has repaired the Casimirs, we recompute the derivatives of C_n for this extended phase space, writing $D_\epsilon = D + \epsilon\phi$ for $\phi \in \mathbb{V}^2_h$, $u_\epsilon = u + \epsilon v$ for $v \in \mathring{\mathbb{V}}^1_h$, $Z'_\epsilon = Z' + \epsilon\gamma'$ for $\gamma' \in (\mathring{\mathbb{V}}^0_h)^\perp$, and defining $q_\epsilon \in \mathbb{V}^0_h$ and $\mathring{Z} \in \mathring{\mathbb{V}}^0_h$ such that

$$\langle \gamma, q_\epsilon D_\epsilon \rangle - \langle \gamma, f + Z'_\epsilon + \mathring{Z}_\epsilon \rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}^0_h, \tag{7.92}$$

$$\langle \gamma, \mathring{Z}_\epsilon \rangle - \langle \nabla^\perp\gamma, u_\epsilon \rangle = 0 \quad \text{for all } \gamma \in \mathring{\mathbb{V}}^0_h. \tag{7.93}$$

Then, for $n \in (1, 2)$,

$$\begin{aligned}
\delta C_n &= \left\langle \frac{\delta C_n}{\delta u}, v \right\rangle + \left\langle \frac{\delta C_n}{\delta D}, \phi \right\rangle + \left\langle \frac{\delta C_n}{\delta Z'}, \gamma' \right\rangle \\
&= \lim_{\epsilon\to 0} \frac{1}{\epsilon}(C_n[u + \epsilon v, D + \epsilon\phi, Z' + \epsilon\gamma'] - C_n[u, D]) \\
&= \int_\Omega \frac{\mathrm{d}}{\mathrm{d}\epsilon}\Big|_{\epsilon=0} D_\epsilon q_\epsilon^n \,\mathrm{d}x \\
&= \left\langle q_\epsilon^{n-1}\big|_{\epsilon=0}, \frac{\mathrm{d}}{\mathrm{d}\epsilon}\Big|_{\epsilon=0} D_\epsilon q_\epsilon \right\rangle + \left\langle (n-1)q_\epsilon^{n-2}\big|_{\epsilon=0} \frac{\mathrm{d}}{\mathrm{d}\epsilon}\Big|_{\epsilon=0} q_\epsilon, D_\epsilon q_\epsilon \right\rangle \\
&= n\left\langle q_\epsilon^{n-1}\big|_{\epsilon=0}, \frac{\mathrm{d}}{\mathrm{d}\epsilon}\Big|_{\epsilon=0} D_\epsilon q_\epsilon \right\rangle - \left\langle (n-1)q_\epsilon^{n}\big|_{\epsilon=0}, \frac{\mathrm{d}}{\mathrm{d}\epsilon}\Big|_{\epsilon=0} D_\epsilon \right\rangle \\
&= n\left\langle q^{n-1}, \gamma' + \frac{\mathrm{d}}{\mathrm{d}\epsilon}\Big|_{\epsilon=0} \mathring{Z}_\epsilon \right\rangle - \langle (n-1)q^n, \phi \rangle \\
&= n\left\langle \mathring{P}_0^\perp q^{n-1}, \gamma' \right\rangle + n\left\langle \mathring{P}_0 q^{n-1}, \frac{\mathrm{d}}{\mathrm{d}\epsilon}\Big|_{\epsilon=0} \mathring{Z}_\epsilon \right\rangle - \langle (n-1)q^n, \phi \rangle \\
&= n\left\langle \mathring{P}_0^\perp q^{n-1}, \gamma' \right\rangle + n\left\langle \nabla^\perp \mathring{P}_0 q^{n-1}, v \right\rangle - \langle (n-1)q^n, \phi \rangle,
\end{aligned} \tag{7.94}$$

where $\mathring{P}_0^\perp$ is the L^2 projection onto the orthogonal subspace to $\mathring{\mathbb{V}}^0_h$. Hence

$$\frac{\delta C_n}{\delta u} = n\nabla^\perp \mathring{P}_0 q^{n-1}, \quad \frac{\delta C_n}{\delta Z'} = n\mathring{P}_0^\perp q^{n-1}, \quad \frac{\delta C_n}{\delta D} = -(n-1)P_2(q^n) \tag{7.95}$$

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for $n \in (1,2)$. Then

$$\begin{aligned}
\{C_n, G\} &= \left\langle q, n\nabla^\perp\left(\mathring{P}_0 q^{n-1}\right) \cdot \frac{\delta G}{\delta u}^\perp \right\rangle \\
&\quad - \Bigg\langle \underbrace{\nabla \cdot n\nabla^\perp\left(\mathring{P}_0 q^{n-1}\right)}_{=0}, \frac{\delta G}{\delta D} \Bigg\rangle + \left\langle \nabla \cdot \frac{\delta G}{\delta u}, -(n-1)P_2(q^n) \right\rangle \\
&\quad + \left\langle \nabla n \mathring{P}_0^\perp q^{n-1}, q\frac{\delta G}{\delta u} \right\rangle - \left\langle \nabla \frac{\delta G}{\delta Z'}, n\nabla^\perp\left(\mathring{P}_0 q^{n-1}\right) \right\rangle \\
&= \left\langle q, n\nabla \underbrace{\left(\mathring{P}_0 q^{n-1} + \mathring{P}_0^\perp q^{n-1}\right)}_{=q^{n-1}} \cdot \frac{\delta G}{\delta u} \right\rangle \\
&\quad - \Bigg\langle \underbrace{\nabla \cdot n\nabla^\perp q^{n-1}}_{=0}, \frac{\delta G}{\delta D} \Bigg\rangle + \left\langle \nabla \cdot \frac{\delta G}{\delta u}, -(n-1)P_2(q^n) \right\rangle \\
&\quad + \Bigg\langle \underbrace{\nabla^\perp \cdot \nabla \frac{\delta G}{\delta Z'}}_{=0}, n\left(\mathring{P}_0 q^{n-1}\right) \Bigg\rangle \\
&= -\left\langle (n-1)\nabla q^n, \frac{\delta G}{\delta u} \right\rangle + \left\langle \nabla \cdot \frac{\delta G}{\delta u}, -(n-1)q^n \right\rangle \\
&= \left\langle (n-1)q^n, \nabla \cdot \frac{\delta G}{\delta u} \right\rangle - \left\langle \nabla \cdot \frac{\delta G}{\delta u}, (n-1)q^n \right\rangle = 0,
\end{aligned} \tag{7.96}$$

where we have repeatedly used $q^n \in \mathbb{V}_h^0$ for $n \in (1,2)$. The surface integral vanished in the penultimate line since $\mathring{P}_0 q^{n-1} \in \mathring{\mathbb{V}}_h^0$ vanishes on the boundary, and the surface integral vanished in the final line since the normal component of $\delta G/\delta u \in \mathring{\mathbb{V}}_h^1$ vanishes on the boundary. Hence the total vorticity C_1 and the enstrophy C_2 are both Casimirs and are conserved by the dynamics.

Bauer and Cotter (2018) demonstrated through numerical experiments that this scheme produces convergent solutions. This idea is closely related to the approach of Ketefian and Jacobson (2009), who introduced vorticity variables at the boundary to make an energy–enstrophy conserving staggered finite difference method.

7.7. Thermal shallow water equations

The thermal shallow water equations provide a useful stepping stone between the rotating shallow water equations and three-dimensional models. This is because they incorporate an additional advected tracer, the temperature, whilst remaining in the two-dimensional setting. Additionally, they provide an interesting reduced model for describing some atmospheric processes, especially when further augmented with a moisture variable, as discussed in the excellent book by Zeitlin (2018). The variational derivation of these equations originates from Ripa (1993),

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and can be placed in the framework of Euler–Poincaré equations by treating the buoyancy s as an additional advected quantity satisfying

$$s_t + u \cdot \nabla s = 0. \tag{7.97}$$

Then the equations take the form

$$\frac{\partial u}{\partial t} + u \cdot \nabla u + f u^{\perp} + s \nabla (D + b) + \frac{D}{2} \nabla s = 0, \tag{7.98}$$

$$\frac{\partial D}{\partial t} + \nabla \cdot (D u) = 0, \tag{7.99}$$

$$\frac{\partial s}{\partial t} + u \cdot \nabla s = 0, \tag{7.100}$$

where u is the horizontal velocity and D is the layer thickness as before. Instead of s, one can work with the buoyancy density $S = sD$, which satisfies

$$S_t + \nabla \cdot (uS) = 0. \tag{7.101}$$

As a consequence of the variational derivation, these equations have Poisson bracket formulations. When S is used as the prognostic variable, the equations can be obtained from the Poisson bracket

$$\{F, G\}_S = \{F, G\}_0 + \left\langle \frac{\delta F}{\delta S}, \nabla \cdot \left(s \frac{\delta G}{\delta u} \right) \right\rangle - \left\langle \frac{\delta G}{\delta S}, \nabla \cdot \left(s \frac{\delta F}{\delta u} \right) \right\rangle, \tag{7.102}$$

where $\{\cdot, \cdot\}_0$ is the Poisson bracket presented in (7.39), combined with the Hamiltonian

$$H = \int_{\Omega} \frac{D|u|^2}{2} + S \left(\frac{D}{2} + b \right) \mathrm{d}x. \tag{7.103}$$

This Poisson bracket formulation has Casimirs of the form

$$C[D, u, S] = \int_{\Omega} D q A \left(\frac{S}{D} \right) + D B \left(\frac{S}{D} \right) \mathrm{d}x, \tag{7.104}$$

where A and B are arbitrary functions.

Alternatively, when s is used as the prognostic variable, we have the following Poisson bracket formulation:

$$\{F, G\}_s = \{F, G\}_0 - \left\langle \nabla \frac{\delta F}{\delta s}, s \frac{\delta G}{\delta u} \right\rangle + \left\langle \nabla \frac{\delta G}{\delta s}, s \frac{\delta F}{\delta u} \right\rangle, \tag{7.105}$$

$$H = \int_{\Omega} \frac{D|u|^2}{2} + D s \left(\frac{D}{2} + b \right) \mathrm{d}x. \tag{7.106}$$

Similarly, this Poisson bracket formulation has Casimirs of the form

$$C[D, u, s] = \int_{\Omega} D q A(s) + D B(s) \, \mathrm{d}x. \tag{7.107}$$

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The advantage of the S formulation is that conservation of total buoyancy,

$$B = \int_\Omega S \, \mathrm{d}x, \tag{7.108}$$

is naturally incorporated, and local conservation is possible when choosing $S \in \mathbb{V}_h^2$. In both cases, for a conforming discretization, $s \in H^1$ is required, that is, we should take $s \in \mathbb{V}_h^0$. In the case of the S formulation, following the approach to q in McRae and Cotter (2014), Eldred *et al.* (2019) proposed introducing $s \in \mathbb{V}_h^0$ as a diagnostic quantity defined by

$$\int_\Omega \gamma D s \, \mathrm{d}x = \int_\Omega \gamma S \, \mathrm{d}x \quad \text{for all } s \in \mathbb{V}_h^0. \tag{7.109}$$

Alternatively, a non-conforming discretization can be obtained by introducing additional facet terms into the Poisson bracket; we shall discuss this further in Section 7.13.

In the case of the conforming S formulation with $S \in \mathbb{V}_h^2$ and prognostic $s \in \mathbb{V}_h^0$, the variational derivatives of H with respect to $u \in \mathbb{V}_h^1$, $D \in \mathbb{V}_h^2$ and $S \in \mathbb{V}_h^2$ become

$$\frac{\delta H}{\delta u} = m \coloneqq P_1(uD), \quad \frac{\delta H}{\delta D} = P_2(|u|^2/2) + S/2, \quad \frac{\delta H}{\delta S} = \frac{D}{2} + b. \tag{7.110}$$

Picking $F = \langle u, w\rangle + \langle \phi, D\rangle + \langle S, \alpha\rangle$ and using the Poisson bracket (7.102) then gives the system of equations

$$\begin{aligned}
&\langle w, u_t\rangle + \langle w, q m^\perp\rangle \\
&- \left\langle \nabla\cdot w, \frac{|u|^2}{2} + \frac{S}{2}\right\rangle - \left\langle \frac{D}{2} + b, \nabla\cdot(sw)\right\rangle = 0 \quad \text{for all } w \in \mathbb{V}_h^1, && (7.111)\\
&\langle \phi, D_t\rangle + \langle \phi, \nabla\cdot m\rangle = 0 \quad \text{for all } \phi \in \mathbb{V}_h^2, && (7.112)\\
&\langle \alpha, S_t\rangle + \langle \alpha, \nabla\cdot(sD)\rangle = 0 \quad \text{for all } \alpha \in \mathbb{V}_h^2, && (7.113)\\
&\langle \gamma, qD\rangle - \langle \nabla^\perp\gamma, u\rangle - \langle \gamma, f\rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}_h^0, && (7.114)\\
&\langle \beta, sD\rangle - \langle \beta, S\rangle = 0 \quad \text{for all } \beta \in \mathbb{V}_h^0. && (7.115)
\end{aligned}$$

The introduction of the thermal variable breaks the symmetry that makes C_n a Casimir for $n > 1$ for the shallow water equations. However, straightforward calculations show that mass M, total buoyancy B and total vorticity Z are all Casimirs for this discrete bracket.

A similar conforming discretization obtained from the Poisson bracket (7.105) also preserves all three of these quantities, with the variation that now B is a quadratic functional

$$B = \int_\Omega sD \, \mathrm{d}x, \tag{7.116}$$

so requires a time integrator that preserves quadratic Casimirs.

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Eldred *et al.* (2019) introduced these formulations plus a number of non-conforming versions with facet integrals. They introduced time integration methods that conserve the relevant Casimirs and demonstrated all of these schemes in convergence tests and other benchmarks.

7.8. Rotating compressible Euler equations

Using the approaches described in this section, Poisson bracket discretizations are possible for any variational fluid model with a Hamiltonian being a function of velocity u, density D and a thermal field θ (as well as extensions to magnetic flux B, for example). In this section we briefly discuss such discretizations for the compressible Euler equations that are the basis for atmospheric dynamical cores in weather and climate models. These equations are given (in the 'θ-Π' formulation) by

$$u_t + (u \cdot \nabla)u + 2\Omega \times u + c_p \theta \nabla \Pi = -g\hat{z}, \tag{7.117}$$

$$\theta_t + u \cdot \nabla \theta = 0, \tag{7.118}$$

$$D_t + \nabla \cdot (uD) = 0, \tag{7.119}$$

$$\Pi^{(1-\kappa)/\kappa} = \frac{R}{p_0} D\theta, \tag{7.120}$$

where u is the velocity, Ω is the rotation vector for the Earth, θ is the potential temperature (a scaling of temperature that absorbs the changes in temperature due to changes in pressure), Π is the Exner function, g is the acceleration due to gravity, $\hat{z}$ is the unit vector pointing away from the centre of the Earth, D is the density, $\kappa = R/c_p$, R is the ideal gas constant, $c_p = R + c_v$ is the specific heat at constant pressure, c_v is the specific heat at constant volume and p_0 is a reference pressure used to define θ.

One Poisson bracket formulation for these equations based around the three-dimensional vorticity vector $\omega = \nabla \times u + 2\Omega$ is

$$\begin{aligned}\{F, G\} = &\left\langle \frac{\delta F}{\delta u}, \omega \times \frac{\delta G}{\delta u} \right\rangle + \left\langle \frac{\delta F}{\delta D}, \nabla \cdot \frac{\delta G}{\delta u} \right\rangle + \left\langle \frac{1}{D} \frac{\delta F}{\delta \theta} \nabla \theta, \frac{\delta G}{\delta u} \right\rangle \\ &- \left\langle \frac{\delta G}{\delta D}, \nabla \cdot \frac{\delta F}{\delta u} \right\rangle - \left\langle \frac{1}{D} \frac{\delta G}{\delta \theta} \nabla \theta, \frac{\delta F}{\delta u} \right\rangle,\end{aligned} \tag{7.121}$$

with Hamiltonian

$$H = \int_\Omega \frac{D|u|^2}{2} + Dgz + \underbrace{c_v D\theta\Pi}_{\text{thermal energy}} \, \mathrm{d}x, \tag{7.122}$$

where z is the height above some reference altitude. Other Poisson bracket formulations are also possible, notably with $\Theta = D\theta$ instead of θ, but we do not intend to be encyclopaedic here.

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Similarly to the treatment of the thermal shallow water equations, a conforming discretization requires that $\theta \in H^1$, that is, we should take $\theta \in \mathbb{W}_h^0$. We take $u \in \mathbb{W}_h^2$, $D \in \mathbb{W}_h^3$. The discrete variational derivatives of H are then

$$\frac{\delta H}{\delta u} = m := P_2(Du), \tag{7.123}$$

$$\frac{\delta H}{\delta D} = P_3\left(\frac{1}{2}|u|^2 + gz + c_p\theta\Pi\right), \tag{7.124}$$

$$\frac{\delta H}{\delta \theta} = c_p P_0(D\Pi), \tag{7.125}$$

where the derivatives of the internal energy, the third term in H, require a little algebra. Using the Poisson bracket (7.121) as the basis for a discretization requires an approximation of $\nabla \times u$ since $\mathbb{W}_h^2$ is not a curl-conforming space. Analogously to (7.54), we approximate $\omega \in \mathbb{W}_h^1$ such that

$$\langle v, \omega\rangle - \langle \nabla \times v, u\rangle = 0 \quad \text{for all } v \in \mathbb{W}_h^1, \tag{7.126}$$

for the case of a domain without boundaries. When boundaries are present, as indeed they must be since the gravitational potential energy term Dgz does not work if the domain is periodic in the vertical, then we must again define $\mathring{\mathbb{W}}_h^1$ as

$$\mathring{\mathbb{W}}_h^1 = \left\{\omega \in \mathbb{W}_h^1 : \omega \times n = 0 \text{ on } \partial\Omega\right\}, \tag{7.127}$$

where n is the outward-pointing normal to Ω. Then the state space must be extended to include $Z' \in (\mathring{\mathbb{W}}_h^1)^\perp$, the L^2-orthogonal complement to $\mathring{\mathbb{W}}_h^1$ in $\mathbb{W}_h^1$, which represents vorticity components on the boundary which have their own dynamics consistent with the conservation of total vorticity. We ignore this aspect for now, but return to it in Section 8.6.

This construction leads to the discretization

$$\langle w, u_t\rangle + \langle w, \omega \times m\rangle - \left\langle \nabla \cdot w, \frac{1}{2}|u|^2 + gz + c_p\theta\Pi\right\rangle - \left\langle w, \frac{1}{D}s\nabla\theta\right\rangle = 0 \quad \text{for all } w \in \mathbb{W}_h^2, \tag{7.128}$$

$$\langle \phi, D_t + \nabla \cdot m\rangle = 0 \quad \text{for all } \phi \in \mathbb{W}_h^3, \tag{7.129}$$

$$\langle \gamma, \theta_t\rangle + \left\langle \gamma\frac{1}{D}\alpha\nabla\theta, m\right\rangle = 0 \quad \text{for all } \gamma \in \mathbb{W}_h^0, \tag{7.130}$$

$$\langle r, m - uD\rangle = 0 \quad \text{for all } r \in \mathbb{W}_h^2, \tag{7.131}$$

$$\langle v, \omega\rangle - \langle \nabla \times v, u\rangle = 0 \quad \text{for all } v \in \mathbb{W}_h^1, \tag{7.132}$$

$$\langle \alpha, s - c_p D\Pi\rangle = 0 \quad \text{for all } \alpha \in \mathbb{W}_h^0, \tag{7.133}$$

$$\Pi^{(1-\kappa)/\kappa} = \frac{R}{p_0}D\theta. \tag{7.134}$$

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In this formulation, there is no approximation in the definition of Π. The equations have non-polynomial terms due to the fractional powers in the definition of Π, which cannot be integrated exactly. This can be dealt with by replacing the exact integral in the definition of the variational derivatives with a quadrature rule. Care must be taken to use this quadrature rule consistently in all of the terms to obtain an energy conserving formulation. In contrast to $\delta H/\delta D$, it is not possible to remove the projection P_θ in the definition of $\delta H/\delta\theta$ from the equations, because $\delta H/\delta\theta$ does not appear in an inner product with a function from $\mathbb{V}_h^0$. Hence we have to introduce a third auxiliary variable s. Lee and Palha (2021) used a related formulation to build a discretization using mimetic spectral elements.

Focusing on the approximation of the pressure gradient term $c_p\theta\nabla\Pi$, the relevant terms are

$$-\langle\nabla\cdot w, c_p\theta\Pi\rangle - \left\langle w, \frac{1}{D}s\nabla\theta\right\rangle = -\langle\nabla\cdot(\theta w), c_p\Pi\rangle + \left\langle w, \left(c_p\Pi - \frac{1}{D}s\right)\nabla\theta\right\rangle, \tag{7.135}$$

which is a consistent approximation to $c_p\theta\nabla\Pi$ since s/D only differs from $c_p\Pi$ by multiplication by D, projection to $\mathbb{W}_h^0$ and division by D again.

As discussed earlier in this article, it can be preferable to use the temperature space $\mathbb{W}_\theta$ for θ, which is more compatible with hydrostatic balance. Since $\mathbb{W}_\theta$ allows discontinuities in the horizontal direction, we need to modify the Poisson bracket formulation to incorporate the non-conforming discretization. This is done by focusing on the following term in the Poisson bracket:

$$\left\langle \frac{1}{D}\frac{\delta F}{\delta\theta}\nabla\theta, \frac{\delta G}{\delta u}\right\rangle = \left\langle \frac{\delta F}{\delta\theta}, \frac{1}{D}\frac{\delta G}{\delta u}\cdot\nabla\theta\right\rangle, \tag{7.136}$$

which leads to the term in (7.130) approximating $u\cdot\nabla\theta$. To adapt this to the partially discontinuous space $\mathbb{W}_\theta$, we replace it with the discontinuous Galerkin discretization

$$L\left[\frac{\delta G}{\delta u}, \frac{\delta F}{\delta\theta}; \theta\right] = -\left\langle \nabla_h\cdot\left(\frac{1}{D}\frac{\delta G}{\delta u}\frac{\delta F}{\delta\theta}\right), \theta\right\rangle + \left\langle\!\!\left\langle \left[\!\left[\frac{1}{D}\frac{\delta G}{\delta u}\frac{\delta F}{\delta\theta}\right]\!\right], \{\theta\}\right\rangle\!\!\right\rangle_\Gamma, \tag{7.137}$$

using the discontinuous Galerkin notation as introduced in Section 4. Here we have chosen a centred flux $\{\theta\}$ but will discuss upwind fluxes in Section 7.13. As usual, this is a consistent approximation with the facet integrals vanishing when u, D, θ, etc., are all smooth functions. Then we use L in a modified Poisson bracket,

$$\begin{aligned}\{F, G\} = &\left\langle \frac{\delta F}{\delta u}, \omega\times\frac{\delta G}{\delta u}\right\rangle + \left\langle \frac{\delta F}{\delta D}, \nabla\cdot\frac{\delta G}{\delta u}\right\rangle + L\left[\frac{\delta G}{\delta u}, \frac{\delta F}{\delta\theta}; \theta\right]\\ &- \left\langle \frac{\delta G}{\delta D}, \nabla\cdot\frac{\delta F}{\delta u}\right\rangle - L\left[\frac{\delta F}{\delta u}, \frac{\delta G}{\delta\theta}; \theta\right].\end{aligned} \tag{7.138}$$

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This leads to the modified velocity equation

$$\langle w, u_t\rangle + \langle w, \omega \times m\rangle - \left\langle \nabla\cdot w, \frac{1}{2}|u|^2 + gz + c_p\theta\Pi\right\rangle + \left\langle \nabla_h \cdot \left(\frac{1}{D}ws\right), \theta\right\rangle - \left\langle\!\!\left\langle \left[\!\left[\frac{1}{D}ws\right]\!\right], \{\theta\}\right\rangle\!\!\right\rangle_\Gamma = 0 \quad \text{for all } w \in \mathbb{W}_h^2, \tag{7.139}$$

in which we recognize another consistent approximation of the pressure gradient term. This concept for introducing any chosen θ advection scheme into a Poisson bracket formulation was introduced in Gassmann and Herzog (2008), with application to a global finite difference model in Gassmann (2013).

Here we should note that formulating a Poisson time integrator for this system is challenging, because the integrands are non-polynomial. As noted to us by Chris Eldred, and implemented in Wimmer, Cotter and Bauer (2021), a Poisson integrator must be approximated by using an incomplete quadrature rule in the time-averaged variational derivatives. This can be done to high order at the expense of a more complicated assembly.

7.9. Upwinding for incompressible Euler: SUPG

One of the interesting and useful features of the Poisson bracket formulation is that it can be modified to incorporate stabilization of the transport schemes whilst remaining antisymmetric and hence energy conserving. In the context of two-dimensional incompressible turbulence (and geostrophic turbulence), this is useful because energy cascades to large scales (where functions can be well approximated by finite element functions) whilst enstrophy cascades to small scales (where they cannot). In energy–enstrophy conserving schemes, vorticity features pile up at the gridscale, leading to unphysical noise, when really they should be cascading to scales below the gridscale. Here a scheme that conserves energy whilst dissipating enstrophy at the small scale through upwind stabilization is appropriate. In three-dimensional isotropic turbulence, energy is also cascading towards small scales, and so additional dissipative gridscale closures or parametrizations are necessary. If these are added to a Poisson bracket formulation with upwind stabilization, we know that there are no spurious energy transfers between scales and between potential, kinetic and internal energy, and the only energy changes are due to the additional dissipative closures and parametrizations. If desired, the energy dissipated from those terms can be collected and recycled into subgrid closures, as is done in Gassmann (2013).

First we discuss energy conserving upwinding techniques for the advection term in the velocity equation. For incompressible quasigeostrophic models, Sadourny and Basdevant (1985) proposed a subgrid closure within the Arakawa Jacobian finite difference formulation by replacing $q \to q - \tau u\cdot\nabla u$ in the Poisson bracket, where τ is a chosen timescale. This provides upwinding by approximating the

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value of q taken upstream along the streamline passing through the gridpoint, hence the name anticipated potential vorticity method (APVM). This was included in a rotating shallow water formulation by Arakawa and Hsu (1990), and has been included in more recent unstructured grid formulations in Ringler *et al.* (2010) and Chen, Gunzburger and Ringler (2012).

When regarded as a numerical scheme instead of a turbulence closure, this modification appears as a $O(\tau)$ consistency error. Instead, in the context of incompressible Euler, one can replace $\omega \to \omega - \tau(\omega_t + u \cdot \nabla\omega)$. Here, the idea is that this term vanishes when the approximation of the solution is accurate and smooth, since then the vorticity equation $\omega_t + u \cdot \nabla\omega = 0$ is well approximated. Hence the approximation is consistent. Following this idea, we can modify the incompressible Euler bracket (7.23) to become

$$\{F, G\} = \int_\Omega (\omega - \tau(\omega_t + u \cdot \nabla\omega)) \frac{\delta F}{\delta u} \cdot \frac{\delta G}{\delta u}^\perp \,\mathrm{d}x, \tag{7.140}$$

where ω is obtained from (7.22) as usual. The discretization becomes

$$\langle w, u_t \rangle + \langle (\omega - \tau(\omega_t + u \cdot \nabla\omega))w, u^\perp \rangle = 0 \quad \text{for all } w \in \zeta_h. \tag{7.141}$$

Writing $u = \nabla^\perp\psi$, $w = \nabla^\perp\phi$ for $\psi, \phi \in \mathbb{V}_h^0$, we get

$$\underbrace{\langle \nabla\phi, \nabla\psi_t \rangle}_{= -\langle \phi, \omega_t \rangle} + \langle (\omega - \tau(\omega_t + u \cdot \nabla\omega))\nabla\phi, u \rangle = 0 \quad \text{for all } \phi \in \mathbb{V}_h^0, \tag{7.142}$$

which we rewrite as

$$\langle \phi + \tau u \cdot \nabla\phi, \omega_t \rangle + \langle \phi + \tau u \cdot \nabla\phi, u \cdot \nabla\omega \rangle = 0 \quad \text{for all } \phi \in \mathbb{V}_h^0, \tag{7.143}$$

after integrating by parts in the term $-\langle \omega\nabla\phi, u \rangle$, which is permissible since $\omega, \phi \in H^1(\Omega)$ and $u \in H(\mathrm{div})$. This is the SUPG discretization of the incompressible Euler equation, which is obtained by replacing the test function ϕ with $\phi + \tau u \cdot \nabla\phi$. The additional term leads to streamwise diffusion of the vorticity ω without harming the consistency of the scheme.

Since the scheme as written here is derived from a Poisson bracket formulation, it conserves energy by construction. Regarding Casimirs C_n, we now get

$$\begin{aligned} \{F, C_n\} &= -n \int_\Omega (\omega + \tau u \cdot \nabla\omega) \frac{\delta F}{\delta u} \cdot \left(\nabla^\perp \omega^{n-1}\right)^\perp \mathrm{d}x \\ &= n \int_\Omega (\omega + \tau u \cdot \nabla\omega) \frac{\delta F}{\delta u} \cdot \nabla\omega^{n-1} \,\mathrm{d}x \\ &= (n-1) \int_\Omega \frac{\delta F}{\delta u} \cdot \nabla\omega^n \,\mathrm{d}x - n\tau \int_\Omega u \cdot \nabla\omega \frac{\delta F}{\delta u} \cdot \left(\nabla^\perp \omega^{n-1}\right)^\perp \mathrm{d}x, \end{aligned} \tag{7.144}$$

and this latter term only vanishes when $n = 1$, hence we have conservation of total vorticity but not enstrophy. By substituting $\phi = \omega$ into (7.143), we can obtain the

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enstrophy dynamics

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \frac{1}{2}\omega^2\,\mathrm{d}x &= \langle \omega, \omega_t\rangle \\ &= \langle (\omega - \tau(\omega_t + u\cdot\nabla\omega))\nabla\omega, u\rangle = 0 \\ &= \underbrace{\left\langle u, \frac{1}{2}\nabla\omega^2\right\rangle}_{=0} - \tau\langle \omega_t, u\cdot\nabla\omega\rangle - \tau\langle u\cdot\nabla\omega, u\cdot\nabla\omega\rangle, \end{aligned} \tag{7.145}$$

where the first term in the last line vanishes after integration by parts and noting that u is divergence-free. The last term is negative semidefinite, and corresponds to diffusion of enstrophy along streamlines, as occurs in APVM. The middle term, which is what we get if we change from APVM to SUPG to ensure consistency of the scheme, is indefinite. However, it only contains one derivative, so it is a lower-order term compared to the streamwise diffusion, and hence the streamwise component of ω is kept smooth.

7.10. Upwinding for incompressible Euler: vorticity-free formulation

An alternative Poisson bracket with upwinding for the two-dimensional incompressible Euler equations stems from the variational formulation of Natale and Cotter (2018), discussed in the previous section. Since that discretization conserves energy, it should not come as a surprise that it has a Poisson bracket formulation, given by

$$\{F, G\} = -\left\langle u, \nabla^\perp\left(\frac{\delta F}{\delta u}^\perp \cdot \frac{\delta G}{\delta u}\right)\right\rangle + \left\langle\!\!\left\langle \{u\}, \left[\!\!\left[n^\perp \cdot \left(\frac{\delta F}{\delta u}^\perp \cdot \frac{\delta G}{\delta u}\right)\right]\!\!\right]\right\rangle\!\!\right\rangle_\Gamma, \tag{7.146}$$

$$H = \frac{1}{2}\int_\Omega |u|^2\,\mathrm{d}x. \tag{7.147}$$

This formulation can be thought of as an alternative way to obtain an approximation to ω when $u \in \mathbb{V}_h^1$. Instead of using an auxiliary equation to define ω, here we integrate the curl by parts in each cell and choose an approximation to u on the facets. This approximation is necessary because although u has continuous normal components, it does not have continuous tangential components; the tangential component of u is multivalued on the boundary. The variational derivation leads to a centred approximation $\{u\}$, but we can equally take an upwind approximation $\tilde{u}$ (where $\tilde{u}$ is the value of u on the upwind side of the facet). This leads to

$$\langle w, u_t\rangle - \langle u, \nabla^\perp(w^\perp\cdot u)\rangle + \langle\!\langle \{u\}, [\![n^\perp\cdot(w^\perp\cdot u)]\!]\rangle\!\rangle_\Gamma = 0 \quad \text{for all } w \in \zeta^\perp. \tag{7.148}$$

It is more difficult to diagnose the enstrophy budget for this scheme than it was for the SUPG scheme. However, numerical experiments in Natale and Cotter (2018) showed that this scheme does indeed tend to reduce enstrophy whilst exactly conserving energy. They also proved convergence of the upwinded scheme, albeit at

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a suboptimal rate; numerical experiments showed convergence at the rate expected given the degree of the polynomials (i.e. second-order L^2 convergence for BDM_1).

7.11. *Scale selective dissipation*

Natale and Cotter (2017) investigated the ability of the schemes in Sections 7.9 and 7.10 to produce energy backscatter from small to large scales consistently with two-dimensional turbulence in the forced dissipative setting.

For the scheme of Section 7.10 they provided a multiscale interpretation of the discretization, in the case of the BDM_1 space (the approach is general for BDM spaces, but discussion is simplified by just describing the lowest-order case). Since $\mathbb{V}_h^1 = BDM_1$ contains $\mathbb{V}_h^{1,l} = \mathrm{P1}^2$ (the space of vector-valued continuous piecewise linear functions) as a subspace, we can write an L^2 orthogonal decomposition,

$$\mathbb{V}_h^1 = \mathbb{V}_h^{1,l} \oplus \mathbb{V}_h^{1,s}, \tag{7.149}$$

where $\mathbb{V}_h^{1,s}$ is the L^2 orthogonal complement of $\mathbb{V}_h^{1,l}$ in $\mathbb{V}_h^1$. Since $\mathbb{V}_h^{1,l}$ is a continuous finite element space and therefore contains functions that are smoother than $\mathbb{V}_h^{1,s}$, we can consider $\mathbb{V}_h^{1,l}$ to be a subspace of larger-scale fields whilst $\mathbb{V}_h^{1,s}$ contains the small scales. This decomposition is not compatible with the decomposition $\mathbb{V}_h^1 = \zeta \oplus \zeta^\perp$, so we have to use the mixed formulation where the divergence-free condition is enforced explicitly via the pressure gradient term. The formulation may be written as

$$\langle v, u_t \rangle + a(u; u, v) + s(u; u, v) - \langle P, \nabla \cdot v \rangle = 0 \quad \text{for all } v \in \mathbb{V}_h^1, \tag{7.150}$$

$$\langle \nabla \cdot u, \phi \rangle = 0 \quad \text{for all } \phi \in \mathbb{V}_h^0, \tag{7.151}$$

where

$$a(\hat{u}; u, v) = \langle \hat{u}^\perp, \nabla(u^\perp \cdot v) \rangle - \langle\!\langle \{\hat{u}^\perp\} \cdot n_+ [\![u^\perp \cdot v]\!] \rangle\!\rangle_\Gamma, \tag{7.152}$$

$$s(\hat{u}; u, v) = -\langle\!\langle c_+ [\![\hat{u}^\perp]\!] \cdot n_+ [\![u^\perp \cdot v]\!] \rangle\!\rangle_\Gamma, \tag{7.153}$$

noting that we use $\hat{u} = u$ in (7.150), and where c_+ is equal to 1 if $u \cdot n_+ \geq 0$ and 0 otherwise.

If we now write $u = u^l + u^s$, with $u^l \in \mathbb{V}_h^{1,l}$ and $u^s \in \mathbb{V}_h^{1,s}$, we observe that

$$\begin{aligned}
s(u; u, u^l) &= -\langle\!\langle c_+ [\![u^\perp]\!] \cdot n_+, [\![u^\perp \cdot u^l]\!] \rangle\!\rangle_\Gamma \\
&= -\langle\!\langle c_+ [\![u^\perp]\!] \cdot n_+, [\![u^\perp]\!] \cdot u^l \rangle\!\rangle_\Gamma \\
&= -\langle\!\langle c_+ [\![u^\perp \cdot n_+]\!], [\![u^\perp \cdot n_+]\!] n_+ \cdot u^l \rangle\!\rangle_\Gamma \\
&= -\langle\!\langle c_+ [\![u^\perp \cdot n_+]\!] n_+, n_+ [\![u^\perp \cdot n_+]\!] n_+ \cdot u^l \rangle\!\rangle_\Gamma \\
&= -\langle\!\langle c_+ [\![u^\perp]\!], [\![u^\perp]\!] n_+ \cdot u^l \rangle\!\rangle_\Gamma \\
&= -\langle\!\langle c_+ [\![u]\!], [\![u]\!] n_+ \cdot u^l \rangle\!\rangle_\Gamma,
\end{aligned} \tag{7.154}$$

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where we used $[\![u^\perp]\!] = [\![u^\perp \cdot n_+]\!] n_+$ since $u^\perp$ has continuous tangential components. Consequently,

$$\begin{aligned} s(u; u, u^s) &= -\langle\!\langle c_+ [\![u^\perp]\!] \cdot n_+, [\![u^\perp \cdot u^s]\!] \rangle\!\rangle_\Gamma \\ &= -\langle\!\langle c_+ [\![u^\perp]\!] \cdot n_+, [\![u^\perp]\!] \cdot (u - u^l) \rangle\!\rangle_\Gamma \\ &= \langle\!\langle c_+ [\![u^\perp]\!] \cdot n_+, [\![u^\perp]\!] \cdot u^l \rangle\!\rangle_\Gamma - \langle\!\langle c_+ [\![u^\perp]\!] \cdot n_+, \underbrace{[\![u^\perp \cdot u]\!]}_{=0} \rangle\!\rangle_\Gamma \\ &= \langle\!\langle c_+ [\![u]\!], [\![u]\!] n_+ \cdot u^l \rangle\!\rangle_\Gamma. \end{aligned} \tag{7.155}$$

Since $\langle u^l, u^s \rangle = 0$, we can obtain equations for the evolution of $E^l = \|u^l\|^2/2$ and $E^s = \|u^s\|/2$ by setting $v = u^l$ and $v = u^s$, respectively:

$$\frac{\mathrm{d}E^l}{\mathrm{d}t} + a\left(u; u, u^l\right) - \left\langle p, \nabla \cdot u^l \right\rangle = \left\langle\!\!\left\langle c_+ u^l \cdot n_+ [\![u]\!], [\![u]\!] \right\rangle\!\!\right\rangle_\Gamma, \tag{7.156}$$

$$\frac{\mathrm{d}E^s}{\mathrm{d}t} + a(u; u, u^s) - \langle p, \nabla \cdot u^s \rangle = -\left\langle\!\!\left\langle c_+ u^l \cdot n_+ [\![u]\!], [\![u]\!] \right\rangle\!\!\right\rangle_\Gamma. \tag{7.157}$$

Since $c_+ u^l \cdot n_+ \geq 0$, the upwinding creates an energy transfer from small to large scales.

Natale and Cotter (2017) demonstrated that this leads to energy backscatter in practice, by using the analysis technique of Thuburn *et al.* (2014*b*). This technique involves simulating two-dimensional incompressible turbulence with Newtonian damping and wavenumber 16 forcing. The instantaneous rate of change of local energy is computed, and then Fourier-transformed to obtain $(\partial/\partial t)E(k)$, the rate of change of energy at wavenumber E. Then the same solution is filtered by removing all wavenumbers above a cut-off k_T, and the rate of change of energy is recomputed using this filtered solution, to obtain $(\partial/\partial t)E_T(k)$. Then the rate of change of subgrid energy $E_{SG}(k) = (\partial/\partial t)E(k) - (\partial/\partial t)E_T(k)$ is computed. This shows the rate of change of energy at wavenumber k due to wavenumbers $> k_T$. This can then be compared with a high-resolution reference solution that has a much larger range of scales from which to support backscatter. This computation is then repeated using enstrophy instead of energy, obtaining $Z_{SG}(k)$. Natale and Cotter (2017) examined the upwind scheme of Natale and Cotter (2018), together with the SUPG scheme (7.141), using this technique, as well as comparing the upwind momentum flux formulation of Guzmán *et al.* (2017), which does not conserve energy. The experiments showed that all three schemes exhibit the trough in $Z_{SG}(k)$ near $k = k_T$, which demonstrates that enstrophy is being transported to smaller scales, consistent with the enstrophy cascade. However, the upwind momentum flux formulation showed no peak at low k in $E_{SG}(k)$ that is indicative of the energy inverse cascade in the reference solution. Both the Natale and Cotter (2018) and SUPG schemes showed such a peak, although it is stronger and closer to the reference solution for the SUPG scheme. When the upwinding is replaced

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by centred approximation in the Natale and Cotter (2018) scheme, and when the τ parameter is set to zero in the SUPG scheme, no statistical equilibrium is reached and the implicit solvers for the systems eventually fail. Hence we conclude that energy conservation and some form of stabilization by upwinding or SUPG are both critical to obtaining these important features in two-dimensional forced dissipative turbulence.

7.12. Upwinding for rotating shallow water equations using potential vorticity

Following Arakawa and Hsu (1990), McRae and Cotter (2014) demonstrated that an energy conserving, enstrophy dissipating scheme for the rotating shallow water equations is possible using the APVM technique where q is replaced by $q - \tau u \cdot \nabla q$ in (7.39), extending the APVM idea discussed above to the rotating shallow water equations. This was demonstrated to have a beneficial effect on the smoothness of the solution whilst still preserving energy. Natale and Cotter (2018) proposed replacing q in (7.39) by $q - \tau((Dq)_t + \nabla\cdot(mq))/D$ (or equivalently by $q - \tau(q_t + m\cdot\nabla q)$, since $D_t + \nabla \cdot m = 0$ in L^2) in order to obtain streamwise stabilization within a consistent scheme, since smooth solutions of the rotating shallow water equations satisfy $(Dq)_t + \nabla \cdot (Duq) = 0$. This leads to the system

$$\begin{aligned}
&\langle w, u_t\rangle + \langle (q - \tau(q_t + m \cdot \nabla q)w, m^\perp\rangle \\
&\qquad - \left\langle \nabla \cdot w, \frac{1}{2}|u|^2 + g(D + b)\right\rangle = 0 \quad \text{for all } w \in \mathbb{V}^1_h, && (7.158)\\
&\qquad \langle \phi, D_t\rangle + \langle \nabla \cdot m\rangle = 0 \quad \text{for all } \phi \in \mathbb{V}^2_h, && (7.159)\\
&\langle \gamma, qD\rangle + \langle \nabla^\perp \gamma, u\rangle - \langle \gamma, f\rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}^0_h, && (7.160)\\
&\qquad \langle v, m - uD\rangle = 0 \quad \text{for all } v \in \mathbb{V}^1_h. && (7.161)
\end{aligned}$$

To obtain the enstrophy dynamics, we use $w = \nabla^\perp q$ in (7.158) and substitute with $\gamma = q$ in (7.160) to obtain

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \frac{1}{2}q^2 D\,\mathrm{d}x &= \langle (q - \tau(q_t + m \cdot \nabla q)), m \cdot \nabla q\rangle \\
&= -\langle \tau(qD)_t m \cdot \nabla q\rangle - \langle \nabla \cdot (qm)), m \cdot \nabla q\rangle, && (7.162)
\end{aligned}$$

where we again have an indefinite consistency term and a streamwise diffusion term that is always ≤ 0. The energy conservation and stabilization of enstrophy, with decay of enstrophy when gridscale features arise through vortex stretching, was demonstrated for this upwind stabilized rotating shallow water scheme in Bauer and Cotter (2018) using numerical experiments.

The enrichment of this scheme with upwind stabilization presents an opportunity for a stability analysis which seems attainable at the time of writing but is currently open. In particular, it would be interesting to consider the stability of a backward Euler step for these equations.

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7.13. Upwind discontinuous Galerkin methods for active tracers

Inspired by the observation of Gassmann and Herzog (2008) that upwinding for advected quantities (such as layer depth, density, temperature, etc.) can be incorporated into an energy conserving scheme by simply ensuring that the antisymmetry is maintained in the bracket, Wimmer, Cotter and Bauer (2020, 2021) examined energy conserving tracer upwinding using upwind discontinuous Galerkin schemes and SUPG schemes, respectively. Wimmer *et al.* (2020) considered upwind discontinuous Galerkin schemes for the rotating shallow water equations, applied to both the layer depth (which is in $\mathbb{V}_h^2$, thus allowing arbitrary discontinuities between cells) and the velocity (which is in $\mathbb{V}_h^1$, and hence allows discontinuity in the tangential components, which is sufficient to allow for some dissipation of small-scale enstrophy).

The goal is to obtain an energy conserving formulation for which the layer depth equation takes the upwind discontinuous Galerkin form

$$\langle \phi, D_t \rangle - \langle \nabla\phi, Du \rangle + \langle\!\langle [\![\phi u]\!], \tilde{D} \rangle\!\rangle_\Gamma = 0 \quad \text{for all } \phi \in \mathbb{V}_h^2. \tag{7.163}$$

To do this, we have to realize it as a modification of the component of the Poisson bracket given by

$$\left\langle \frac{\delta F}{\delta D}, \nabla \cdot \frac{\delta H}{\delta u} \right\rangle, \tag{7.164}$$

where $\delta F/\delta u = \phi$ and $\delta H/\delta u = P_1(Du)$. The problem is that u explicitly appears in (7.163), whilst $\delta H/\delta u$ involves a projection of uD. Wimmer *et al.* (2020) solved this problem by introducing a recovery operator $\mathcal{U}\colon (D, m) \in \mathbb{V}_h^2 \times \mathbb{V}_h^1 \to u \in \mathbb{V}_h^1$ defined by

$$\langle Dv, u \rangle = \langle v, m \rangle \quad \text{for all } v \in \mathbb{V}_h^1, \tag{7.165}$$

which is well-defined provided that $D > 0$ (breaking this condition will cause the scheme to fail in any case). Note in particular that if $m = P_1(Dw)$ for any $w \in \mathbb{V}_h^1$, then $\mathcal{U}(D, m) = w$.

Thus we can rewrite (7.163) as

$$\left\langle \frac{\delta F}{\delta D}, D_t \right\rangle \underbrace{- \left\langle \nabla \frac{\delta F}{\delta D}, D\mathcal{U}\left(D, \frac{\delta H}{\delta u}\right) \right\rangle + \left\langle\!\!\left\langle \left[\!\!\left[\frac{\delta F}{\delta D} \mathcal{U}\left(D, \frac{\delta H}{\delta u}\right) \right]\!\!\right], \tilde{D} \right\rangle\!\!\right\rangle_\Gamma}_{} = 0 \tag{7.166}$$

for all $\delta F/\delta D \in \mathbb{V}_h^2$, with the term marked by the underbrace replacing (7.164). In order to keep the bracket antisymmetric, we also make the same substitutions in the corresponding term with F and G exchanged, and the Poisson bracket becomes

$$\begin{aligned} \{F, G\} = &\left\langle \frac{\delta F}{\delta u}, q \frac{\delta G}{\delta u}^\perp \right\rangle - \left\langle \nabla \frac{\delta F}{\delta D}, D\mathcal{U}\left(D, \frac{\delta G}{\delta u}\right) \right\rangle + \left\langle\!\!\left\langle \left[\!\!\left[\frac{\delta F}{\delta D} \mathcal{U}\left(D, \frac{\delta G}{\delta u}\right) \right]\!\!\right], \tilde{D} \right\rangle\!\!\right\rangle_\Gamma \\ &+ \left\langle \nabla \frac{\delta G}{\delta D}, D\mathcal{U}\left(D, \frac{\delta G}{\delta u}\right) \right\rangle - \left\langle\!\!\left\langle \left[\!\!\left[\frac{\delta G}{\delta D} \mathcal{U}\left(D, \frac{\delta F}{\delta u}\right) \right]\!\!\right], \tilde{D} \right\rangle\!\!\right\rangle_\Gamma. \end{aligned} \tag{7.167}$$

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The velocity upwinding used is a development of the Natale and Cotter (2018) scheme, which does not require an auxiliary potential vorticity variable. To achieve this, we apply the modification in the q term of the Poisson bracket,

$$\left\langle \frac{\delta F}{\delta u}, q\frac{\delta G}{\delta u}\right\rangle \mapsto \left\langle \frac{\delta F}{\delta u}, \frac{1}{D}\nabla^\perp\cdot u\frac{\delta G}{\delta u}^\perp\right\rangle + \left\langle \frac{\delta F}{\delta u}, \frac{f}{D}\frac{\delta G}{\delta u}^\perp\right\rangle. \tag{7.168}$$

Following a discontinuous Galerkin methodology, we then integrate by parts separately in each cell, and select $\tilde{u}$, the value of u from the upwind side, in the corresponding facet integral, to obtain

$$-\left\langle u, \nabla^\perp\left(\frac{\delta F}{\delta u}\cdot\frac{1}{D}\frac{\delta G}{\delta u}^\perp\right)\right\rangle + \left\langle\!\!\left\langle \tilde{u}, \left[\!\left[n^\perp\cdot\left(\frac{\delta F}{\delta u}\cdot\frac{1}{D}\frac{\delta G}{\delta u}^\perp\right)\right]\!\right]\right\rangle\!\!\right\rangle_\Gamma. \tag{7.169}$$

Since we are already using $\mathcal{U}$ in the layer depth terms, we might as well avoid additional projections and use it to replace $(\delta G/\delta u)/D$. Putting all of this together gives

$$\begin{aligned}\{F,G\} = &-\left\langle u, \nabla^\perp\left(D\mathcal{U}\left(D,\frac{\delta F}{\delta u}\right)\cdot\mathcal{U}\left(D,\frac{\delta G}{\delta u}\right)^\perp\right)\right\rangle\\ &+\left\langle\!\!\left\langle \tilde{u}, \left[\!\left[n^\perp\cdot\left(D\mathcal{U}\left(D,\frac{\delta F}{\delta u}\right)\cdot\mathcal{U}\left(D,\frac{\delta G}{\delta u}\right)^\perp\right)\right]\!\right]\right\rangle\!\!\right\rangle_\Gamma\\ &-\left\langle \nabla\frac{\delta F}{\delta D}, D\mathcal{U}\left(D,\frac{\delta G}{\delta u}\right)\right\rangle + \left\langle\!\!\left\langle \left[\!\left[\frac{\delta F}{\delta D}\mathcal{U}\left(D,\frac{\delta G}{\delta u}\right)\right]\!\right], \tilde{D}\right\rangle\!\!\right\rangle_\Gamma\\ &+\left\langle \nabla\frac{\delta G}{\delta D}, D\mathcal{U}\left(D,\frac{\delta F}{\delta u}\right)\right\rangle - \left\langle\!\!\left\langle \left[\!\left[\frac{\delta G}{\delta D}\mathcal{U}\left(D,\frac{\delta F}{\delta u}\right)\right]\!\right], \tilde{D}\right\rangle\!\!\right\rangle_\Gamma. \end{aligned}\tag{7.170}$$

Now, if we use this Poisson bracket to generate the dynamical equations for D and u, we get

$$\begin{aligned}&\langle w, u_t\rangle - \langle u, \nabla^\perp(D\mathcal{U}(D,w)\cdot u^\perp)\rangle\\ &\quad+\langle\!\langle \tilde{u}, [\![Dn^\perp\cdot(\mathcal{U}(D,w)\cdot u^\perp)]\!]\rangle\!\rangle_\Gamma\\ &+\left\langle \nabla\frac{\delta H}{\delta D}, D\mathcal{U}(D,w)\right\rangle - \left\langle\!\!\left\langle \left[\!\left[\frac{\delta H}{\delta D}\mathcal{U}(D,w)\right]\!\right], \tilde{D}\right\rangle\!\!\right\rangle_\Gamma = 0 \quad \text{for all } w\in\mathbb{V}_h^1, \end{aligned}\tag{7.171}$$

$$\langle \phi, D_t\rangle - \langle\nabla\phi, Du\rangle + \langle\!\langle [\![\phi u]\!], \tilde{D}\rangle\!\rangle_\Gamma = 0 \quad \text{for all } \phi\in\mathbb{V}_h^2, \tag{7.172}$$

which conserves energy by construction, despite the presence of the upwind terms. As written, it is not clear how to implement this scheme, due to the presence of the application of $\mathcal{U}$ to the test function w. It is not scalable to compute and store $\mathcal{U}(D,w)$ for each test function w, since $\mathcal{U}(D,w)$ is globally supported in general. Wimmer *et al.* (2020) solved this problem by introducing an auxiliary variable $r\in\mathbb{V}_h^1$ such that

$$\begin{aligned}\langle r, Dv\rangle = &-\langle u, \nabla^\perp(Dv\cdot u^\perp)\rangle\\ &+\langle\!\langle \tilde{u}, [\![Dn^\perp\cdot(v\cdot u^\perp)]\!]\rangle\!\rangle_\Gamma \quad \text{for all } v\in\mathbb{V}_h^1. \end{aligned}\tag{7.173}$$

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Then

$$\begin{aligned}\langle r, w\rangle &= \langle r, \mathcal{U}(D, w)D\rangle \\ &= -\langle u, \nabla^\perp(D\mathcal{U}(D, w)\cdot u^\perp)\rangle \\ &\quad + \langle\!\langle \tilde{u}, [\![Dn^\perp \cdot (\mathcal{U}(D, w)\cdot u^\perp)]\!]\rangle\!\rangle_\Gamma \quad \text{for all } w \in \mathbb{V}_h^1, \end{aligned} \tag{7.174}$$

as required. Hence we obtain the three coupled equations for

$$\left(u, r, D, \frac{\delta H}{\delta D}\right) \in \mathbb{V}_h^1 \times \mathbb{V}_h^1 \times \mathbb{V}_h^2 \times \mathbb{V}_h^2, \tag{7.175}$$

where

$$\langle w, u_t\rangle - \langle Dw, r\rangle = 0 \quad \text{for all } w \in \mathbb{V}_h^1, \tag{7.176}$$

$$\begin{aligned}&\langle r, v\rangle - \langle u, \nabla^\perp(Dv\cdot u^\perp)\rangle + \langle\!\langle \tilde{u}, [\![Dn^\perp \cdot (v\cdot u^\perp)]\!]\rangle\!\rangle_\Gamma \\ &\qquad + \left\langle \nabla\frac{\delta H}{\delta D}, Dv\right\rangle - \left\langle\!\!\left\langle \left[\!\!\left[\frac{\delta H}{\delta D} v\right]\!\!\right], \tilde{D}\right\rangle\!\!\right\rangle_\Gamma = 0 \quad \text{for all } v \in \mathbb{V}_h^1, \end{aligned} \tag{7.177}$$

$$\langle \phi, D_t\rangle - \langle \nabla\phi, Du\rangle + \langle\!\langle [\![\phi u]\!], \tilde{D}\rangle\!\rangle_\Gamma = 0 \quad \text{for all } \phi \in \mathbb{V}_h^2, \tag{7.178}$$

$$\left\langle s, \frac{\delta H}{\delta D} - \frac{1}{2}|u|^2 - gD\right\rangle = 0 \quad \text{for all } s \in \mathbb{V}_h^2. \tag{7.179}$$

Note that the use of upwinding in the D equation has altered the $\delta H/\delta D$ term in the u equation, and it now appears in terms other than an inner product with $\nabla\cdot w$. This means we have to solve for the projection to $\mathbb{V}_h^1$ in an additional equation, which complicates the solution of this system after discretization with an implicit Poisson integrator (which is necessary for exact energy conservation for the fully discrete scheme). Wimmer *et al.* (2020) addressed the solution by using a Picard iteration on (u, D), keeping the standard linearization about a state of rest as an update equation and forming the nonlinear residual by first computing $\delta H/\delta D$ and r and substituting them into the residuals for u and D. The linear system can then be solved for using hybridization techniques as described in Section 5. Another possible approach is to apply Newton's method to the full four-component system. Then, when solving the Jacobian linear system for the update, δr and $\delta(\delta H/\delta D)$ can be eliminated as part of a Schur complement preconditioner; the Schur complement in u and D can then be approximated by the corresponding Schur complement arising from a more standard discretization such as those discussed in earlier sections.

Wimmer *et al.* (2020) demonstrated that this scheme combined with a Poisson integrator produces relative energy conservation error of size 10^{-9} after four Picard iterations, when applied to a standard test case used in the development of numerical schemes for numerical weather prediction (the flow over a mountain test case 5 from Williamson *et al.* (1992)). In fact, similar-sized energy errors were even obtained when using the implicit midpoint rule (also approximated using four Picard iterations), showing that the most important aspect of energy conservation is in the spatial discretization, at least for this test problem. Additionally, if a

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midpoint rule is used then there is no need for the additional auxiliary variable r above. This is an example where the reduction in energy error through space and time discretization tricks is lost due to the energy error from doing a finite number of nonlinear iterations.[6]

7.14. SUPG methods for active tracers

Wimmer *et al.* (2021) examined similar approaches when SUPG schemes are applied to the advected quantities. The motivation for this is that an SUPG scheme is required to stabilize the vertical transport of temperature when it is approximated in the $\mathbb{W}_h^\theta$ space proposed in Section 2. SUPG schemes have additional complications as they modify the test function throughout the equation, including in the time derivative term. Wimmer *et al.* (2021) addressed this problem as follows. First, we adopt the notation that SUPG makes the modification $\gamma \mapsto \gamma + \tau S(u;\gamma)$ to the test function $\gamma \in \mathbb{W}_h^\theta$. This general notation is to cover different possibilities; for standard SUPG for continuous finite element spaces the modification takes the form

$$S(u;\gamma) = u \cdot \nabla\gamma. \tag{7.180}$$

We note that $S(u;\gamma)$ will always be linear in the test function γ, but we do not require linearity in the other variables. Then, if the plain version of the discrete transport equation takes the form

$$\langle \gamma, \theta_t \rangle + L(u,\theta;\gamma) = 0 \quad \text{for all } \gamma \in \mathbb{W}_h^\theta, \tag{7.181}$$

then the SUPG version takes the form

$$\langle s + \tau S(u;s), \theta_t \rangle + L(u,\theta; s + \tau S(u;s)) = 0 \quad \text{for all } s \in \mathbb{W}_h^\theta. \tag{7.182}$$

For example, with a standard continuous Galerkin approximation, we would have

$$L(u,\theta;\gamma) = -\langle \nabla\gamma, u\theta \rangle \quad \text{for all } \gamma \in \mathbb{W}_h^\theta. \tag{7.183}$$

We then define $s(u;\gamma) \in \mathbb{W}_h^\theta$ according to

$$\langle s(u;\gamma) + \tau S(u; s(u,\gamma)), \sigma \rangle = \langle \gamma, \sigma \rangle \quad \text{for all } \sigma \in \mathbb{W}_h^\theta. \tag{7.184}$$

Wimmer *et al.* (2021) proved the well-posedness of this definition. Our SUPG transport equation then becomes

$$\langle \gamma, \theta_t \rangle + L(u,\theta; s(u;\gamma) + \tau S(u; s(u;\gamma))) = 0 \quad \text{for all } \gamma \in \mathbb{W}_h^\theta. \tag{7.185}$$

Following the principle of Gassmann and Herzog (2008) again, we substitute this form into the relevant terms in the Poisson bracket, which are

$$\{F, G\} = \cdots - \left\langle \frac{1}{D}\frac{\delta G}{\delta \theta}\nabla\theta, \frac{\delta F}{\delta u} \right\rangle + \left\langle \frac{1}{D}\frac{\delta F}{\delta \theta}\nabla\theta, \frac{\delta G}{\delta u} \right\rangle. \tag{7.186}$$

[6] Thanks to Golo Wimmer for pointing out this observation.

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Since we know that $(\delta H/\delta u)/D = u$ in the unapproximated case, the substitution gives

$$\{F, G\} = \cdots - L\left(\frac{1}{D}\frac{\delta G}{\delta u}, \theta; s\left(u; \frac{\delta F}{\delta \theta}\right) + \tau S\left(u; s\left(u; \frac{\delta F}{\delta \theta}\right)\right)\right) + L\left(\frac{1}{D}\frac{\delta F}{\delta u}, \theta; s\left(u; \frac{\delta G}{\delta \theta}\right) + \tau S\left(u; s\left(u; \frac{\delta G}{\delta \theta}\right)\right)\right). \tag{7.187}$$

This produces dynamical equations of the form

$$\left\langle \gamma + \tau S\left(\frac{1}{D}\frac{\delta H}{\delta u}; \gamma\right), \theta_t \right\rangle + L\left(\frac{1}{D}\frac{\delta H}{\delta u}, \theta; \gamma + \tau S\left(\frac{1}{D}\frac{\delta H}{\delta u}; \gamma\right)\right) = 0, \quad \gamma \in \mathbb{W}_\theta, \tag{7.188}$$

$$\langle w, u_t \rangle + \cdots - L\left(\frac{1}{D}w, \theta; s\left(u; \frac{\delta H}{\delta \theta}\right) + \tau S\left(u; s\left(u; \frac{\delta H}{\delta \theta}\right)\right)\right) = 0, \quad w \in \mathbb{W}_h^1,$$

where '$\cdots$' represents the terms coming from the other parts of the Poisson bracket. The latter term in the u_t equation is an approximation of the term

$$-c_p \theta \nabla \Pi, \tag{7.189}$$

in the case of the compressible Euler equations. To replace $(\delta H/\delta u)/D$ in the θ_t equation back with u again, Wimmer *et al.* (2021) also used the $\mathcal{U}$ operator as described above for the shallow water equations, but we will not incorporate that additional complexity here.

Wimmer *et al.* (2021) demonstrated robust upwind stabilization combined with energy conservation in various test problems using this method. For the thermal shallow water equations, the upwinded version demonstrated much smoother temperature fields than in the standard energy conserving version. This is significant because the thermal shallow water equations exhibit very fine structures in the temperature field which lead to the accumulation of numerical noise at the gridscale, if upwinding is not used. For the compressible Euler equations in a vertical slice formulation in a falling bubble configuration, they showed that the energy conserving form of the upwinded scheme leads to the appearance of secondary Kelvin–Helmholtz vortices that appear in much higher-resolution simulations of the same problem (but do not appear with upwinding schemes on the same resolution that do not conserve energy). This latter result seems to suggest that the energy conserving formulation is transferring potential energy dissipated from the upwind transport scheme and injecting it into the kinetic energy in a manner that is consistent with subscale processes in the higher-resolution simulation. Wimmer *et al.* (2021) also developed formulae that showed that the energy conservation is indeed maintained by the transfer of dissipated potential energy into kinetic energy. Since the potential energy dissipation occurs at the gridscale, this raises the concern that the energy conservation leads to the production of noise in the velocity field. By careful measurement of the gridscale component of the velocity field in numerical

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experiments, it was shown that the energy injection is at a larger scale, similar to what was observed by Natale and Cotter (2017). The naïve intuition that the energy conserving formulation balances upwinding diffusion with antidiffusion in the velocity term is incorrect, as the additional terms are not second-order derivatives in velocity.

8. Consistent vorticity and potential vorticity transport

Another subtopic in structure preserving schemes is that of schemes that have consistent vorticity transport. This means that although potential vorticity or vorticity is not one of the prognostic variables, the discretized dynamics imply a discretization for the (potential) vorticity transport equation. This is useful because it can imply additional control on the smoothness of the velocity field, especially when upwinding is incorporated into the implied vorticity dynamics. To quote Ringler *et al.* (2010): 'Given the fundamental importance of PV in geophysical flows, numerical models are sometimes constructed to faithfully represent some aspects of the PV dynamics within the discrete system.' Although this property is closely linked with the Poisson bracket formulations described in Section 7, we have chosen to discuss it in a separate section, because some papers have emphasized the importance of this aspect whilst not strictly building in energy conservation.

The history again comes through the 'C grid' finite difference school of methods for numerical weather prediction, with Sadourny providing key ideas (Sadourny 1972, Sadourny and Basdevant 1985), and more modern application to unstructured grids taking place in Ringler *et al.* (2010).

For the incompressible Euler equations, we start from (7.13). Applying the two-dimensional curl $\nabla^\perp\cdot$ leads to the law of conservation of vorticity,

$$\omega_t + \nabla\cdot(\omega u) = 0, \tag{8.1}$$

from which conservation of the Casimirs C_n can be directly derived. We have already seen in the previous section that the energy conserving discretization (7.24) implies a consistent discretization of (8.1), and that the modification of the bracket (7.140) leads to a consistent SUPG discretization. It is this idea that we seek to translate to the equations of geophysical fluid dynamics.

8.1. *Consistent potential vorticity transport in the energy–enstrophy conserving framework*

For the rotating shallow water equations, the starting point is the 'vector-invariant' form, which is

$$u_t + qDu^\perp + g\nabla(D+b) = 0, \tag{8.2}$$

where $q = (\nabla^\perp\cdot u + f)/D$ as before. Applying $\nabla^\perp\cdot$ leads to

$$(qD)_t + \nabla\cdot(qDu) = 0, \tag{8.3}$$

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which is the law of conservation of potential vorticity (from which the conservation of the Casimirs C_n can also be derived directly). Here the identity $\nabla^\perp \cdot \nabla$ is used to eliminate the pressure gradient term $g\nabla(D + b)$ from this conservation law, and so compatible discretizations that preserve this identity are important to maintain this structure.

This occurs straightforwardly in the energy–enstrophy conserving formulation of McRae and Cotter (2014), presented in Section 7.12. Taking $w = -\nabla^\perp \gamma$ for $\gamma \in \mathbb{V}_h^0$ in (7.60) gives

$$\langle -\nabla^\perp \gamma, u_t \rangle - \langle \nabla \gamma, qm \rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}_h^0. \tag{8.4}$$

Then, taking the time derivative of (7.62) and substituting into (8.4) gives

$$\langle \gamma, (qD)_t \rangle - \langle \nabla \gamma, qm \rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}_h^0, \tag{8.5}$$

which is a standard finite element discretization of (8.3). This becomes even clearer after integrating by parts in the second term to obtain

$$\langle \gamma, (qD)_t + \nabla \cdot (qm) \rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}_h^0, \tag{8.6}$$

which is simply the projection of (8.3) into $\mathbb{V}_h^0$. For the compatible finite element discretization, this integration by parts is an identity (provided that $u \cdot n = 0$ on domain boundaries) since $\gamma, q \in \mathbb{V}_h^0 \subset H^1$ and $m \in \mathbb{V}_h^1 \subset H(\mathrm{div})$. If we apply similar manipulations to these in the case of the upwind stabilized system (7.158)–(7.161), we obtain the following stabilized discretization of the potential vorticity conservation law:

$$\langle \gamma, (qD)_t \rangle - \langle \nabla \gamma, mq - \tau m(q_t + m \cdot \nabla q) \rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}_h^0. \tag{8.7}$$

Some rearrangement and integration by parts (using $m \cdot n = 0$ on the boundary) then gives

$$\langle \gamma, (qD)_t + \nabla \cdot (mq) \rangle - \langle \tau m \cdot \nabla \gamma, m \cdot \nabla q \rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}_h^0. \tag{8.8}$$

As we have previously noted, $D_t + \nabla \cdot m = 0$ in L^2, so we can write

$$\left\langle \gamma + \frac{1}{D} \tau m \cdot \nabla \gamma, (qD)_t + \nabla \cdot (mq) \right\rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}_h^0, \tag{8.9}$$

which we observe is an SUPG discretization of the law of conservation of potential vorticity. Even though the potential vorticity is not a prognostic variable, we obtain consistent dynamics for this diagnosed quantity.

Also in a similar direction, Lee (2021) designed a scheme that applies Petrov–Galerkin-style upwinding by evaluating mass flux test functions at downstream locations along advective characteristics (similar to a semi-Lagrangian scheme). This was demonstrated to have a beneficial effect on the implied potential vorticity dynamics (although the scheme does dissipate energy, unlike those described above).

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In the case of the thermal shallow water equations, there is a source term in the potential vorticity equation. Eldred *et al.* (2019) constructed a scheme based on the ideas above so that the diagnostic potential vorticity satisfies a discretized version of this conservation law with sources, which preserves constant potential vorticity in the case when entropy s is constant.

8.2. *Consistent potential vorticity transport using primal–dual grids*

The previous section suggests an approach to designing numerical schemes where one selects an advection scheme for potential vorticity (which could be higher-order accurate, with limiters, etc.). Then the corresponding scheme for velocity that is consistent with the chosen advection scheme is deduced. This makes use of the compatible spaces, since an equation for vorticity can be immediately obtained by choosing a test function $w = \nabla^\perp \gamma$ for $\gamma \in \mathbb{V}_h^0$ in the velocity equation. Thuburn and Cotter (2015) took this approach to designing a compatible scheme based on combinations of spaces on overlaid primal–dual grids, necessitating lowest-order spaces. To raise the order of accuracy of the velocity advection scheme, they chose a third-order upwind finite volume scheme for the potential vorticity on the dual grid (a swept area scheme in this case) to obtain higher-order accurate potential vorticity dynamics in space and time. The advantage of third-order (and, generally, odd-order) transport schemes is that a backward error analysis shows that the leading-order error is diffusive rather than dispersive: this reduces gridscale oscillations in the numerical solution. This was achieved by considering both the potential vorticity and velocity equations after time discretization. This was possible because the finite volume scheme can be reinterpreted as an equation of the form (or a discrete-time formulation that is analogous to)

$$\langle \gamma, (qD)_t \rangle - \langle \nabla\gamma, mq^* \rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}_h^0, \tag{8.10}$$

for some chosen q^*, where m is the mass flux such that $D_t + \nabla \cdot m = 0$ in L^2 for the corresponding discrete scheme for D. Then this equation can be obtained from the following velocity equation:

$$\langle w, u_t \rangle + \langle w, q^* m^\perp \rangle + \langle \nabla \cdot w, P \rangle = 0 \quad \text{for all } w \in \mathbb{V}_h^1, \tag{8.11}$$

for some P. This can be checked upon taking $w = \nabla^\perp \gamma$.

8.3. *Consistent potential vorticity transport using Taylor–Galerkin schemes*

In a similar direction, Shipton *et al.* (2018) used a third-order Taylor–Galerkin scheme for the diagnostic potential vorticity equation, and constructed the prognostic velocity equation accordingly. A Taylor–Galerkin scheme is an extension of the Lax–Wendroff technique in which one expands a Taylor series in time, transforming higher-order time derivatives into space derivatives using the advection equation, before discretizing in space to obtain stable schemes.

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8.4. Preservation of constant potential vorticity

Another aspect of these schemes is that although we wish to solve the equation in conservative form (8.10) to conserve total vorticity, the potential vorticity also solves

$$q_t + u \cdot \nabla q = 0, \tag{8.12}$$

obtained by combining (8.3) with the continuity equation for D. This means that the value of q is preserved along characteristics moving at speed u. In particular, it can be desirable that if q is constant then it remains constant, which is a property of (8.12). To obtain this at the discrete level, we need a mass flux m such that $D_t + \nabla \cdot m = 0$. This is straightforward when the scheme (7.61) is used, since one can take $\phi = D_t + \nabla \cdot m$, implying that $D_t + \nabla \cdot m = 0$ in L^2, as we have previously discussed. This becomes more complicated when discontinuous Galerkin methods are used (or finite volume methods for lowest-order spaces, as used in Thuburn and Cotter (2015)), because the equation is not immediately in that form. However, such a form can be deduced using compatible properties of the spaces. Thuburn and Cotter (2015) used such an approach coming from finite volume schemes (Ringler *et al.* 2010), which was translated to discontinuous Galerkin methods by Shipton *et al.* (2018). To describe this, we consider an upwind discontinuous Galerkin method for D:

$$\langle \phi, D_t \rangle - \langle \nabla \phi, Du \rangle + \langle\!\langle [\![\phi u]\!], \tilde{D} \rangle\!\rangle_\Gamma = 0 \quad \text{for all } \phi \in \mathbb{V}_h^2. \tag{8.13}$$

For each cell K, we then define $m \in \mathbb{V}_h^1(K)$ from

$$\int_f \gamma (m - u\tilde{D}) \cdot n \, \mathrm{d}S = 0 \quad \text{for all } \gamma \in T(f),\ f \in K, \tag{8.14}$$

$$\int_K w \cdot (m - uD) \, \mathrm{d}x = 0 \quad \text{for all } w \in \mathbb{V}_h^{1,-}(K), \tag{8.15}$$

where f are all the facets of K, $T(f)$ is the appropriate trace space on f spanned by $u \cdot n|_f$ with $u \in \mathbb{V}_h^1(K)$, and $\mathbb{V}_h^{1,-}(K)$ is the appropriately sized curl-conforming space to close the system, as used in the definition of the commuting projection into $\mathbb{V}_h^1$. For example, if $\mathbb{V}_h^1$ is BDM_k then $\mathbb{V}_h^{1,-}$ is the (rotated) Raviart–Thomas space of degree $k-1$. This is a local projection that can be evaluated independently in each cell K, with $m \in \mathbb{V}_h^1$ (since the normal components agree on facets). Then we have

$$\begin{aligned} \langle \phi, \nabla \cdot m \rangle &= -\langle \nabla \phi, m \rangle + \langle\!\langle [\![\phi]\!], m \rangle\!\rangle_\Gamma \\ &= -\langle \nabla \phi, uD \rangle + \langle\!\langle [\![\phi]\!], u\tilde{D} \rangle\!\rangle_\Gamma \quad \text{for all } \phi \in \mathbb{V}_h^2, \end{aligned} \tag{8.16}$$

where we used that $\phi \in \mathbb{V}_h^2 \implies \nabla \phi \in \mathbb{V}_h^{1,-}$ and $\phi|_f \in T(f)$, following standard calculations defining the commuting projection. Hence we obtain (7.61) with m defined as above, and so $D_t + \nabla \cdot m = 0$ in L^2. We then aim to construct our scheme to have the form (8.10), with the property that $q = 1 \implies q^* = 1$. Then, if $q = 1$,

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we have

$$\begin{aligned}\langle \gamma, Dq_t \rangle &= -\langle \gamma, D_t \rangle + \langle \nabla\phi, m \rangle \\ &= -\langle \gamma, D_t + \nabla \cdot m \rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}_h^0. \end{aligned} \tag{8.17}$$

In other words, we have that q constant implies that q stays constant. Both Thuburn and Cotter (2015) and Shipton *et al.* (2018) implemented this approach in a semi-implicit framework by writing the time-stepping scheme as a fixed number of Picard iterations, taking care to show that the properties above are enforced at each Picard iteration.

8.5. Consistent potential vorticity transport with boundaries

Earlier we discussed the extension in Bauer and Cotter (2018) of the scheme of McRae and Cotter (2014) to the case of the presence of boundaries. This extension also solves the problem of how to obtain a scheme with a consistent discretization for the implied potential vorticity equation in that case, including the use of SUPG stabilization there. Taking the time derivative of (7.88) gives

$$\begin{aligned}\langle \gamma, (qD)_t \rangle &= \left\langle \gamma, \mathring{Z}_t + Z'_t \right\rangle \\ &= \left\langle \mathring{P}_h^1 \gamma, \mathring{Z}_t \right\rangle + \left\langle \mathring{P}_0^\perp \gamma, Z'_t \right\rangle \\ &= \left\langle \nabla^\perp \mathring{P}_h^1 \gamma, u_t \right\rangle + \left\langle \mathring{P}_0^\perp \gamma, Z'_t \right\rangle \\ &= -\left\langle \nabla^\perp \mathring{P}_h^1 \gamma, qm^\perp \right\rangle - \left\langle \nabla \mathring{P}_0^\perp \gamma, qm \right\rangle \\ &= -\langle \nabla\gamma, qm \rangle \quad \text{for all } \gamma \in \mathbb{V}_h^0, \end{aligned} \tag{8.18}$$

as required. Similarly, the equations can be modified so that q is replaced by q^*, the SUPG modified potential vorticity, to obtain a consistent SUPG stabilized diagnostic potential vorticity equation (but we do not discuss it here). The existence of this implied potential vorticity equation actually also provides a useful equivalent formulation that avoids explicit computation of Z' (which is in the rather cumbersome space $\mathring{P}_0^\perp$, which is not efficient to compute with). Rather than separately incrementing Z', we can redundantly increment q on the whole domain, solving

$$\langle w, u_t \rangle + \langle qw, m^\perp \rangle - \left\langle \nabla \cdot w, \frac{1}{2}|u|^2 + g(D+b) \right\rangle = 0 \quad \text{for all } w \in \mathring{\mathbb{V}}_h^1, \tag{8.19}$$

$$\langle \phi, D_t \rangle + \langle \nabla \cdot m \rangle = 0 \quad \text{for all } \phi \in \mathbb{V}_h^2, \tag{8.20}$$

$$\langle \gamma, (qD)_t \rangle + \langle \nabla\gamma, qm \rangle = 0 \quad \text{for all } \gamma \in \mathbb{V}_h^0, \tag{8.21}$$

having initialized q from (7.54). This provides a computationally feasible technique for a scheme with consistent potential vorticity dynamics (and indeed a scheme that conserves energy and even enstrophy if the SUPG form is not used). In a practical implementation, if errors from round-off or truncated numerical solvers cause q and u to diverge from

$$\langle \gamma, qD \rangle + \langle \nabla^\perp \gamma, u \rangle - \langle \gamma, f \rangle = 0 \quad \text{for all } \gamma \in \mathring{\mathbb{V}}_h^0 \tag{8.22}$$

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at any point, then we may replace $q \leftarrow q' + q$, where $q' \in \mathring{\mathbb{V}}^0_h$ satisfies

$$\langle \gamma(q' + q)D \rangle + \langle \nabla^\perp \gamma, u \rangle - \langle \gamma, f \rangle = 0 \quad \text{for all } \gamma \in \mathring{\mathbb{V}}^0_h. \tag{8.23}$$

This is equivalent to solving for the new q from (7.54) with Dirichlet boundary condition obtained from the old q.

8.6. *Consistent vorticity transport in three dimensions*

Following a similar route, we can show that (7.128)–(7.134) have a consistent discretization of vorticity transport. Initially, to see this, assume that there are no boundaries. Then we choose $w = \nabla \times \Sigma$ in (7.134) with $\Sigma \in \mathbb{W}^1_h$. This gives

$$\langle \Sigma, \omega_t \rangle + \langle \nabla \times \Sigma, \omega \times m \rangle - \left\langle \nabla \times \Sigma, \frac{s}{D} \nabla \theta \right\rangle = 0 \quad \text{for all } \Sigma \in \mathbb{W}^2_h, \tag{8.24}$$

where either $s = c_p D\Pi$ or $s = \delta H / \delta \theta$, depending on whether or not the Poisson bracket formulation is used. Equation (8.24) is an integral form of the vorticity equation

$$\omega_t + \nabla \times (\omega \times m) + \nabla \left(\frac{s}{D} \right) \times \nabla \theta = 0. \tag{8.25}$$

The last term on the left-hand side of (8.25) is known as the baroclinic torque. If we dot (8.25) with $\nabla\theta$ and use (5.18), we obtain the potential vorticity conservation law

$$(Dq)_t + \nabla \cdot (qm) = 0, \tag{8.26}$$

where q is the Ertel potential vorticity

$$q = \frac{\omega \cdot \nabla \theta}{D}. \tag{8.27}$$

It would be wonderful to have a discretization that has a consistent conservation of Ertel's potential vorticity, in the manner of this section. This could be done if one could choose test functions $\Sigma = \psi \nabla \theta$ in (8.24) with $\psi \in \mathbb{W}^0_h$, with θ also satisfying an exact advection equation $\theta_t + u \cdot \nabla \theta = 0$ in L^2. Neither of these properties appear to be possible in the present framework, and this remains a challenging unsolved problem. What is possible, if $\theta \in \mathbb{W}^0_h$, is to obtain conservation of total potential vorticity,

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega Dq \, \mathrm{d}x &= \frac{\mathrm{d}}{\mathrm{d}t} \langle \nabla \theta, \omega \rangle \\ &= \langle \nabla \theta_t, \omega \rangle + \langle \nabla \theta, \omega_t \rangle \end{aligned}$$

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$$= -\langle \theta_t, \underbrace{\delta_1 \omega}_{=\delta_1\delta_2 u=0} \rangle + \langle \nabla\theta, \omega_t \rangle$$
$$= -\left\langle \underbrace{\nabla \times \nabla\theta}_{=0}, \omega \times m - \frac{s}{D}\nabla\theta \right\rangle, \tag{8.28}$$

upon choosing $\Sigma = \nabla\theta$. Note that this also works for any quantity $\nabla\psi$ for $\psi \in \mathbb{W}_h^0$, dynamical or not.

Returning to the conservation of vorticity in (8.24), we can develop upwind stabilizations of the vorticity equation using a residual-based approach (similar to that of Bendall and Wimmer (2023)) by replacing

$$\langle \nabla \times \Sigma, \omega \times m \rangle \mapsto \langle \nabla \times \Sigma, \omega^* \times m \rangle, \tag{8.29}$$

where

$$\omega^* = \omega - \tau \left(\omega_t + \nabla \times (\omega \times m) + \nabla\left(\frac{s}{D}\right) \times \nabla\theta \right), \tag{8.30}$$

for a stabilization parameter τ.

This approach can also be extended to the case of domains with boundaries, which of course is important for atmosphere models that have a top and bottom surface, where we assume that the boundary condition is $u \cdot n = 0$. This requires that $u \in \mathring{\mathbb{W}}_h^2$, and we have a difficulty similar to that for the shallow water equations with defining vorticity, since a consistent approximation requires

$$\langle \Sigma, \omega \rangle = \langle \Sigma, 2\Omega \rangle - \langle \nabla \times \Sigma, u \rangle + \langle\langle n \times \Sigma, u \rangle\rangle \quad \text{for all } \Sigma \in \mathbb{W}_h^1, \tag{8.31}$$

and $\omega \in \mathbb{W}_h^1$, not $\mathring{\mathbb{W}}_h^1$. We have the same solution to the difficulty, which is to introduce the space $(\mathring{\mathbb{W}}_h^1)^\perp$, the L^2 complement of $\mathring{\mathbb{W}}_h^1$ in $\mathbb{W}_h^1$, and writing $\omega = \omega' + \mathring{\omega}$, with $\omega' \in \mathring{\mathbb{W}}_h^1$ and $\mathring{\omega} \in \mathring{\mathbb{W}}_h^1$. Then ω' has its own dynamics defined by

$$\langle \Sigma, \omega_t' \rangle + \langle \nabla \times \Sigma, \omega \times m \rangle - \left\langle \nabla \times \Sigma, \frac{1}{D} s \nabla\theta \right\rangle = 0 \quad \text{for all } \Sigma' \in (\mathbb{W}_h^1)^\perp. \tag{8.32}$$

In the Poisson bracket setting, the bracket (7.121) is then extended as

$$\{F, G\} = \cdots + \left\langle \nabla \times \frac{\delta F}{\delta \omega'}, \omega \times \frac{\delta G}{\delta u} - \frac{1}{D}\frac{\delta G}{\delta \theta}\nabla\theta \right\rangle$$
$$- \left\langle \nabla \times \frac{\delta G}{\delta \omega'}, \omega \times \frac{\delta F}{\delta u} - \frac{1}{D}\frac{\delta F}{\delta \theta}\nabla\theta \right\rangle. \tag{8.33}$$

Similar calculations to those in Sections 7.6 and 8.5 then lead from this Poisson bracket to (8.24). Further, just as in Sections 7.6 and 8.5, solving the resulting equation set is equivalent to solving (8.24) in place of (8.31). This type of scheme is as yet not explored in numerical computations.

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9. Structure preserving schemes on non-affine meshes

The interpretation of the compatible finite element discrete de Rham complexes and the finite element exterior calculus (FEEC) is well known. Arnold, Falk and Winther (2006, 2010) and Arnold (2018) provided a comprehensive unifying treatment of the stability and error analysis of numerical approximations of the Hodge Laplacian, which is now finding applications in the design of stable discretizations for the Stokes equation and in elasticity. In applications to geophysical fluid dynamics, one of the main applications of finite element exterior calculus has been in establishing a clean separation between topological and geometric aspects of the formulation. In particular, when non-affine meshes are used, at first sight it seems that it is not possible to perform exact integration when assembling the discrete operators on a computer, because the integrands are non-polynomial. For example, when a function $u \in \mathbb{V}_h^1$ is transformed back to a reference cell, a contravariant Piola transform must be used, so it will take the form $J^{-\top}\hat{u}/\det(J)$, where J is the Jacobian of the transformation from the reference cell to the mesh cell. J is non-constant for non-affine meshes, so $1/\det(J)$ is non-polynomial. In general, this creates potential problems because we rely on clean separation in the Helmholtz decomposition of $\mathbb{V}_h^1$ between divergence-free and rotational components to obtain good long-time behaviour for all methods (not just structure preserving ones). These types of errors have the potential to break structure preserving properties of all the schemes discussed in this section. However, all is not lost, because many of the terms in our fluid dynamics equations result in cancellation of geometric factors (factors involving J when the equations are transformed back to the reference cell). This cancellation of geometric factors can be derived using standard vector calculus, but they are most transparently established under the invariance of various operations involving differential forms under pullback (wedge product, exterior derivative, etc.). In fact, the author of this review only became aware of the possibility of some of them after computing with the differential form formulations. In particular, we have the following formulae:

$$\int_{\hat{K}} \hat{\phi}\hat{u} \cdot \hat{w}^{\perp} \,\mathrm{d}x = \int_K \phi u \cdot w^{\perp} \,\mathrm{d}x, \tag{9.1}$$

$$\int_{\hat{K}} \hat{\phi}\nabla \cdot \hat{w} \,\mathrm{d}x = \int_K \phi \nabla \cdot w \,\mathrm{d}x, \tag{9.2}$$

$$\int_{\hat{f}} \hat{\phi}\hat{u} \cdot \hat{n} \,\mathrm{d}S = \int_f \phi u \cdot n \,\mathrm{d}S, \tag{9.3}$$

where $g_K : \hat{K} \to K$ is the mapping from reference cell $\hat{K}$ to a mesh cell K, $\hat{f}$ is a facet of cell $\hat{K}$ with normal $\hat{n}$, f is the image of $\hat{f}$ under g with normal n, and

$$\hat{\phi} = \phi \circ g, \quad \frac{J\hat{w}}{\det(J)} = w \circ g, \quad \frac{J\hat{u}}{\det(J)} = u \circ g. \tag{9.4}$$

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Following computations in Thuburn and Cotter (2012) for the finite difference case (interpreted as discrete exterior calculus (DEC)), Cotter and Thuburn (2014) presented a finite element exterior calculus formulation in the setting of the family of methods related to McRae and Cotter (2014). Relevant to the discussion of this section, they noted the existence of these Jacobian-free pullback formulae as derived from the properties of pullbacks of differential forms. Eldred and Bauer (2022) provided further insight into this family of DEC and FEEC schemes for rotating shallow water equations. They noted that a special case of the Leibniz rule for the wedge product, in which one of the two terms is a constant, is underpinning the presence of an implied conserved potential vorticity as described in Section 8, and hence the conservation of total vorticity and potential vorticity for associated Poisson bracket schemes.

In the context of the Poisson bracket formulation for rotating shallow water equations, the pullback formulae (9.1)–(9.3) can be used to maintain a structure preserving formulation. This is achieved by replacing the L^2 inner product with a quadrature rule,

$$\langle \phi, p \rangle_q = \sum_i \phi(x_i) q(x_i) w_i, \tag{9.5}$$

and similarly for vector-valued functions. In practice, this quadrature is defined cellwise as usual, as the image of quadrature points on the reference cell $\hat{K}$ under the map g. This incomplete quadrature causes a 'variational crime', and then analysis is required to demonstrate whether the convergence rate is affected; a minimal condition is that it still satisfies the definition of an inner product on the relevant finite element spaces. This modification produces a modified Helmholtz decomposition,

$$\mathbb{V}_h^1 = B_h^1 \oplus \tilde{\mathfrak{h}}_h^1 \oplus (\tilde{B}^*)_h^1, \tag{9.6}$$

where $\tilde{\mathfrak{h}}_h^k$ and $(\tilde{B}^*)_h^k$ are modified spaces constructed using $\tilde{\delta}_k$, the dual operator defined using the modified inner product, that is,

$$\left\langle \phi, \tilde{\delta}_h^k u \right\rangle_q = -\left\langle d^{k+1}\phi, u \right\rangle_q. \tag{9.7}$$

It also produces a modified definition of the variational derivative,

$$\left\langle \frac{\delta F}{\delta u}, v \right\rangle_q = \lim_{\epsilon \to 0} \frac{1}{\epsilon}(F[u + \epsilon v] - F[u]). \tag{9.8}$$

However, we maintain the usual L^2 inner product in (7.39), since all of the terms in the bracket have polynomial integrands when transformed back to the reference cell, and hence can be evaluated exactly. Further, the integrands in (7.54) can also be integrated exactly for similar reasons. If we assume that the modified inner product is exact for these terms as well (it just needs to be a sufficiently high-order

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Gaussian quadrature), then the formulation (7.60)–(7.63) is still energy–enstrophy preserving by the above arguments. This modification of the inner product can be extended to more complicated formulations involving temperature and in three dimensions.

10. Summary and outlook

In this survey we have introduced the application of compatible finite element methods to the world of geophysical fluid dynamics, with applications to oceans, weather and climate. We have introduced the main properties of the spaces and their application to understanding the discrete wave propagation properties when they are used for linearized models. We have discussed how to build compatible finite element methods for nonlinear models, focusing on the transport and pressure gradient terms; we have also discussed the approach to solving the linear and nonlinear systems that arise from certain time-stepping schemes. Then we have surveyed the use of compatible finite element methods in structure preserving methods: variational integrators, Poisson integrators and schemes with consistent potential vorticity transport. There is much more work to be done in the analysis of all of these schemes, considering stability, convergence of solutions, and mesh independence of preconditioners, etc. There are also plenty of research directions in finding practical approaches that incorporate as much of the structure preserving properties as possible. The finite element exterior calculus continues to be an important guiding principle for designing compatible finite element methods for geophysical fluid dynamics. It should prove a useful tool for the rigorous analysis of stability of these methods for fully nonlinear systems, where only limited progress has been made so far. The author looks forward to many fruitful collaborations on compatible finite element methods for geophysical fluid dynamics in the future.

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