

Variational Discretization Framework for Geophysical Flow Models

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Abstract. We introduce a geometric variational discretization framework for geophysical flow models. The numerical scheme is obtained by discretizing, in a structure-preserving way, the Lie group formulation of fluid dynamics on diffeomorphism groups and the associated variational principles. Being based on a discrete version of the Euler-Poincaré variational method, this discretization approach is widely applicable. We present an overview of structure-preserving variational discretizations of various equations of geophysical fluid dynamics, such as the Boussinesq, anelastic, pseudo-incompressible, and rotating shallow-water equations. We verify the structure-preserving nature of the resulting variational integrators for test cases of geophysical relevance. Our framework applies to irregular mesh discretizations in 2D and 3D in planar and spherical geometry and produces schemes that preserve invariants of the equations such as mass and potential vorticity. Descending from variational principles, the discussed variational schemes exhibit a discrete version of Kelvin circulation theorem and show excellent long term energy behavior.

Keywords: Anelastic and pseudo-incompressible equations \cdot Rotating shallow-water equations \cdot Soundproof and compressible fluids \cdot Variational principle \cdot Euler-Poincaré equations \cdot Structure-preserving discretizations

1 Introduction

Variational methods are a powerful tool to derive consistent models from Hamilton's principle of least action. The equations of motion follow by computing the critical curve of the action functional associated to the Lagrangian of the system. When derived from a discrete version of variational principles, the resulting discretizations preserve important geometric properties of their underlying continuous equations, such as long term stability, consistency in statistical properties and conservation of stationary solutions, see e.g. [9, 12, 14].

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Given the generality of the approach, variational methods are applied in various fields of interest. While most of the literature covers variational integrators for ordinary differential equations (ODEs), in recent years they have been developed also for partial differential equations (PDEs), in particular for fluid and geophysical fluid dynamics (GFD), see e.g. [13] and [1-3,6]. The numerical schemes descend from discretizing the Lie group formulation of fluid dynamics on diffeomorphism groups and the associated variational principles.

In the field of GFD, variational integrators are of particular interest given their conservation of invariants which is a crucial property for long time integrations to guarantee accurate representation of the statistical properties of these models [4,7]. In this context, the rotating shallow-water (RSW) equations, both in the plane and on the sphere, have received considerable attention because they allow us to study the essential features of the full 3D equations in an idealized setting. Another interesting approximation of the Euler equations is to filter out sound waves as they are assumed to be negligible for atmospheric models. In this context, mostly anelastic and pseudo-incompressible approximations are studied, cf. [8,11].

Here, we present a unified variational discretization framework that covers both the soundproof approximations of the Euler equations [2,3] and the compressible rotating shallow-water case [1,5]. As shown in Sect. 2, this framework will allow us to stress differences in the description of compressible and incompressible flows. Naturally, the Lie groups approximations describing the different flow models differ from each other, but the derivation of the corresponding Lie algebras and fluid's vector fields follows for all cases the same procedure. In contrast, the treatment of advected quantities differs between soundproof and compressible models. For some of these models, we present in Sect. 3 some numerical results of the schemes from Sect. 2.4 focusing again on the similarities and differences between them. Finally, in Sect. 4 we draw some conclusions.

2 Variational Discretization Framework

The discretization procedure mimics the continuous variational principle step by step. In Table 1 the corresponding continuous definitions are given that have to be suitably approximated.

Recall that in the Lagrangian representation, the variational principle is the Hamilton principle $\delta \int L(\varphi, \dot{\varphi}) dt = 0$ written on the appropriate diffeomorphism group of the fluid domain \mathcal{M} . For instance for the RSW equations the group Diff(\mathcal{M}) of all diffeomorphisms is used, whereas for soundproof models, one chooses the group Diff $_{\bar{\sigma}\mu}(\mathcal{M})$ that preserve a weighted volume $\bar{\sigma} d\mathbf{x}$, with $\bar{\sigma} = 1$, $\bar{\sigma} = \bar{\rho}$, or $\bar{\sigma} = \bar{\rho}\bar{\theta}$, for the Boussinesq, anelastic, or pseudo-incompressible model, in which $\bar{\rho}(z)$ and $\bar{\theta}(z)$ characterize vertically varying reference states for density and potential temperature, respectively, in hydrostatic balance [2].

The variational principle inherited from the Hamilton principle in Eulerian (spatial) representation is the Euler-Poincaré principle ([10]). The spatial Lagrangian is expressed in terms of the Eulerian velocity \mathbf{u} , the fluid depth

h, and/or the potential temperature θ , and the fluid equations follow from $\delta \int_0^T \ell dt = 0$ with respect to constrained variations $\delta \mathbf{u}$, δh or $\delta \theta$, see Table 1.

2.1 Discrete Diffeomorphism Groups

The discretization procedure starts with the choice of a discrete version of the diffeomorphism group, [1,13], obtained by first discretizing the space of functions $\mathcal{F}(\mathcal{M})$ on which the group acts by composition on the right, and then identifying a finite dimensional group acting by matrix multiplication on the finite dimensional space of discrete functions, while preserving some properties of the action by diffeomorphisms (constant functions are preserved). Given a mesh \mathbb{M} of \mathcal{M} and choosing as discrete functions the space \mathbb{R}^N of piecewise constant functions on \mathbb{M} , this results in the following matrix groups:

- for compressible flow: $D(\mathbb{M}) = \{q \in GL(N)^+ \mid q \cdot \mathbf{1} = \mathbf{1}\}$, with $\mathbf{1} = (1, ..., 1)^T$, in which the condition $q \cdot \mathbf{1} = \mathbf{1}$ encodes, at the discrete level, the fact that constant functions are preserved under composition by a diffeomorphism;
- for soundproof flow: $D_{\bar{\sigma}}(\mathbb{M}) = \{q \in \mathrm{GL}(N)^+ \mid q \cdot \mathbf{1} = \mathbf{1} \text{ and } q^T \Omega^{\bar{\sigma}} q = \Omega^{\bar{\sigma}} \},\$ with $\Omega_i^{\bar{\sigma}} := \int_{C_i} \bar{\sigma}(z) d\mathbf{x}$, for a cell C_i , and where the additional constraint imposes the preservation of the weighted volume at the discrete level.

The action of the groups $\mathsf{D}(\mathbb{M})$ and $\mathsf{D}_{\bar{\sigma}}(\mathbb{M})$ by matrix multiplication on discrete functions $F \in \mathbb{R}^N$ is denoted as

$$F \in \mathbb{R}^N \mapsto qF = F \circ q^{-1} \in \mathbb{R}^N, \quad q \in \mathsf{D}(\mathbb{M}), \tag{1}$$

where the suggestive notation $F \circ q^{-1}$ for the multiplication of the vector F by the matrix q is introduced to indicate that this action is understood as a discrete version of the action of $\text{Diff}(\mathcal{M})$ and $\text{Diff}_{\bar{\sigma}}(\mathcal{M})$ by composition on $\mathcal{F}(\mathcal{M})$. The situation is formally illustrated by the diagram

$$f \in \mathcal{F}(\mathcal{M}) \xrightarrow{\text{Diff}(\mathcal{M}) \text{ or Diff}_{\bar{\sigma}}(\mathcal{M})} f \circ \varphi^{-1} \in \mathcal{F}(\mathcal{M})$$

$$\downarrow \text{Discretization} \qquad \qquad \downarrow \text{Discretization}$$

$$F \in \mathbb{R}^{N} \xrightarrow{\mathsf{D}(\mathbb{M}) \text{ or } \mathsf{D}_{\bar{\sigma}}(\mathbb{M})} q \cdot F \in \mathbb{R}^{N}$$

2.2 Discrete Lie Algebra and Discrete Vector Fields

By taking the derivative of continuous and discrete actions at the identity, we get $\frac{d}{dt}\Big|_{t=0} f \circ \varphi_t^{-1} = -\mathbf{d}f \cdot \mathbf{u}$ and $\frac{d}{dt}\Big|_{t=0} F \circ q_t^{-1} = AF$, where $\frac{d}{dt}\Big|_{t=0} \varphi_t = \mathbf{u}$ and $\frac{d}{dt}\Big|_{t=0} q_t = A$. Hence AF, with A an element of the Lie algebra of $\mathsf{D}(\mathbb{M})$ or $\mathsf{D}_{\bar{\sigma}}(\mathcal{S})$ is a discretization of (minus) the derivative of f in the direction \mathbf{u} . The Lie algebras of $\mathsf{D}(\mathbb{M})$ and $\mathsf{D}_{\bar{\sigma}}(\mathcal{S})$ are:

- for compressible flow: $\mathfrak{d}(\mathbb{M}) = \{A \in \operatorname{Mat}(N) \mid A \cdot \mathbf{1} = 0\},\$
- for soundproof flow: $\mathbf{\mathfrak{d}}_{\bar{\sigma}}(\mathbb{M}) = \{A \in \operatorname{Mat}(N) \mid A \cdot \bar{\mathbf{1}} = 0, A^{\mathsf{T}} \Omega^{\bar{\sigma}} + \Omega^{\bar{\sigma}} A = 0\}.$

However, not all $A \in \mathfrak{d}(\mathbb{M})$ or $\mathfrak{d}_{\bar{\sigma}}(\mathbb{M})$ can be interpreted as discrete vector fields. This induces *nonholonomic constraints* on the Lie algebras which have to be appropriately taken into account in the variational principle.

Nonholonomic Constaints. For both *soundproof* and *compressible* fluids it is required that fluxes are nonzero only between neighboring cells, hence we have the linear constraint $S = \{A \in \mathfrak{d}(\mathbb{M})/\mathfrak{d}_{\sigma}(\mathbb{M}) \mid A_{ij} = 0, \forall j \notin N(i)\}$ where N(i) is the set of indices of those cells adjacent to cell *i*.

For the compressible case, we have the additional constraint, $\Omega_{ii}A_{ij} = -\Omega_{jj}A_{ji}$, for all $j \neq i$, where $\Omega = \Omega^{\bar{\sigma}}$ with $\bar{\sigma} = 1$. This gives the additional linear constraint $\mathcal{R} = \{A \in \mathfrak{d}(\mathbb{M}) \mid A^{\mathsf{T}}\Omega + \Omega A \text{ is diagonal}\}$. These nonholonomic constraints are taken into account by using the Euler–Poincaré–d'Alembert principle, which is the nonholonomic version of the Euler–Poincaré principle.

Discrete Vector Fields. Taking into account these nonholonomic constraints, it can be shown that if a matrix Aapproximates a vector field \mathbf{u} , then,



- for compressible flow: matrix elements of $A \in \mathcal{S} \cap \mathcal{R}$ satisfy $A_{ij} \simeq -\frac{1}{2\Omega_{ii}} \int_{D_{ij}} (\mathbf{u} \cdot \mathbf{n}_{ij}) dS, \quad A_{ii} \simeq \frac{1}{2\Omega_{ij}} \int_{\Omega_{ij}} (\operatorname{div} \mathbf{u}) d\mathbf{x}.$
- $\frac{1}{2\Omega_{ii}} \int_{C_i} (\operatorname{div} \mathbf{u}) d\mathbf{x},$ - for soundproof flow: matrix elements of $A \in \mathcal{S}$ satisfy $A_{ij} \simeq -\frac{1}{2\Omega^{\overline{c}}} \int_{D_{ii}} (\bar{\sigma} \, \mathbf{u} \cdot \mathbf{n}_{ij}) dS,$

Fig. 1. Flux associated to A_{ij} .

for all $j \in N(i)$, $j \neq i$, with D_{ij} the hyperface common to cells C_i and C_j and \mathbf{n}_{ij} is the normal vector on D_{ij} pointing from C_i to C_j , cf. Fig. 1.

Discrete Advected Quantities. To formulate the discrete Euler–Poincaré– d'Alembert principle, we need to define appropriate actions of $D(\mathbb{M})$ on discrete fluid depth D for RSW and of $D_{\bar{\sigma}}(\mathbb{M})$ on discrete potential temperature Θ for SP. In both cases, the action results from the definition in (1), namely

- for compressible flow: D is a discrete density so the action, $D \mapsto D \bullet q$, is dual to the action on discrete functions: $\langle D \bullet q, F \rangle = \langle D, F \circ q^{-1} \rangle$ for all $F \in \mathbb{R}^N$, with respect to the discrete L^2 pairing. It results in $D \bullet q = \Omega^{-1}q^{\mathsf{T}}\Omega D$.
- for soundproof flow: Θ is a discrete function so the action is $q\Theta = \Theta \circ q^{-1}$ as in (1). Then, $\Theta(t) = q(t)\Theta_0$.

2.3 Euler–Poincaré–d'Alembert (EPA) Variational Principle

Consider the spatial discrete Lagrangian $\ell_d = \ell_d(A, Q) : \mathfrak{d}(\mathbb{M})/\mathfrak{d}_{\bar{\sigma}}(\mathbb{M}) \times \mathbb{R}^N \to \mathbb{R}$ with $Q \in \mathbb{R}^N$ an advected quantity, $(D \text{ or } \Theta)$. The discrete EPA principle reads: $\delta \int_0^T \ell_d(A, Q) dt = 0$ for variations $\delta A = \partial_t B + [B, A], B(0) = B(T) = 0$, and

- for compressible flow: $\delta Q = -Q \bullet B$, with $A, B \in S \cap \mathcal{R}$,
- for soundproof flow: $\delta Q = BQ$, with $A, B \in S$.

Case 1: soundproof model. The discrete EPA principle, with $Q = \Theta$, yields the following semidiscrete equations for $(A(t), \Theta(t)) \in \mathfrak{d}_{\bar{\sigma}}(\mathbb{M}) \times \mathbb{R}^N$, [2]:

$$\left(\frac{d}{dt}\frac{\delta\ell_d}{\delta A} + \left[\frac{\delta\ell_d}{\delta A}\Omega^{\bar{\sigma}}, A\right](\Omega^{\bar{\sigma}})^{-1} + \left(\Theta\frac{\delta\ell_d}{\delta\Theta}^{\mathsf{T}}\right)^{(A)} + dP\right)_{ij} = 0, \text{ for all } i \in N(j)$$
(2)

for some discrete function P (the discrete pressure). Here $(dP)_{ij} = P_j - P_i$ and ()^(A) denotes the skew-symmetric part of a matrix.

Case 2: compressible model. The discrete EPA principle, with Q = D, yields the following semidiscrete equations for $(A(t), D(t)) \in \mathfrak{d}(\mathbb{M}) \times \mathbb{R}^N$, [1]:

$$\mathbf{P}\left(\frac{d}{dt}\frac{\delta\ell}{\delta A} + \Omega^{-1}\left[A^{\mathsf{T}}, \Omega\frac{\delta\ell}{\delta A}\right] + D\frac{\delta\ell}{\delta D}^{\mathsf{T}}\right)_{ij} = 0, \quad \text{for all } i \in N(j), \qquad (3)$$

where **P** is the projection associated to the nonholonomic constraint, [1]. These equations are accompanied with the discrete continuity equation $\frac{d}{dt}D + D \bullet A = 0$.

We provide in Table 1 a summary that enlightens the correspondence between the continuous and discrete objects. Note that in both cases, the resulting equations of motion for soundproof and compressible flows are valid on any reasonable mesh (e.g. not degenerated cells [1]). To result in implementable code, we have to choose a mesh and a suitable discrete flat operators such as in [13].

Table 1. Conti	inuous and d	iscrete object	ts for so	undproof	(SP) and	compressible	(CP)
discretizations.	The diverge	nce is denote	d by div	7 and the	Jacobian	by J .	

Continuous diffeomorphisms	Discrete diffeomorphisms				
$\operatorname{Diff}(\mathcal{M}) \ni \varphi$	$D(\mathbb{M}) \ni q$				
Group action on functions	Group action on discrete functions				
$f \mapsto f \circ \varphi^{-1}$	$F \mapsto F \circ q^{-1} =: qF$				
Group action on densities	Group action on discrete densities				
CP: $h \mapsto h \bullet \varphi = (h \circ \varphi) J \varphi$	CP: $D \mapsto D \bullet q = \Omega^{-1} q^{T} \Omega D$				
Eulerian velocity and advected quantity	Disc. Eulerian veloc. and advec. quantity				
$\mathbf{u} = \dot{\varphi} \circ \varphi^{-1}, \begin{cases} \text{SP:} \theta = \Theta_0 \circ \varphi^{-1} \\ \text{CP:} h = (h_0 \circ \varphi^{-1}) J \varphi^{-1} \end{cases}$	$A = \dot{q}q^{-1}, \begin{cases} \text{SP:} \Theta = q\Theta_0\\ \text{CP:} D = \Omega^{-1}q^{-T}\Omega D_0 \end{cases}$				
Euler-Poincaré principle	Euler-Poincaré-d'Alembert principle				
$\delta \int_0^T \ell(\mathbf{u}, h/\theta) dt = 0, \delta \mathbf{u} = \partial_t \mathbf{v} + [\mathbf{v}, \mathbf{u}]$	$\delta \int_0^T \ell(A, D/\Theta) dt = 0, \delta A = \partial_t B + [B, A]$				
$\int SP: \delta\theta = -\mathbf{d}\theta \cdot \mathbf{v}$	$\int SP: \delta\Theta = B\Theta, \qquad A, B \in \mathcal{S}$				
CP: $\delta h = -\operatorname{div}(h\mathbf{v})$	$\begin{cases} CP: & \delta D = -\Omega^{-1} B^{T} \Omega D, & A, B \in \mathcal{S} \cap \mathcal{R} \end{cases}$				

2.4 Numerical Schemes on Irregular Simplicial Meshes

The numerical schemes are obtained from (2) and (3), by specializing them to the chosen mesh and the chosen discrete Lagrangian, which requires the construction of a discrete "flat" operator $A \in S \cap \mathcal{R} \mapsto A^{\flat}$ associated to the given mesh, see [13]. For instance, for the RSW case the discrete Lagrangian is

$$\ell_d(A,D) = \frac{1}{2} \sum_{i,j=1}^N D_i A_{ij}^{\flat} A_{ij} \Omega_{ii} + \sum_{i,j=1}^N D_i R_{ij}^{\flat} A_{ij} \Omega_{ii} - \frac{1}{2} \sum_{i=1}^N g(D_i + B_i)^2 \Omega_{ii}.$$
(4)

The discrete flat operator is defined from the two conditions $A_{ij}^{\flat} = 2\Omega_{ii} \frac{h_{ij}}{f_{ij}} A_{ij}$, and $A_{ij}^{\flat} + A_{jk}^{\flat} + A_{ki}^{\flat} = K_j^e \langle \omega(A^{\flat}), \zeta_e \rangle$, for $i, k \in N(j), k \notin N(i)$, with e the node common to cells C_i, C_j, C_k , where $K_k^e := \frac{|\zeta_e \cap C_k|}{|\zeta_e|}, \langle \omega(A^{\flat}), \zeta_e \rangle := \sum_{h_{mn} \in \partial \zeta_e} A_{mn}^{\flat}$, and where $|\zeta_e \cap C_k|$ is the area of the intersection of C_k with the dual cell ζ_e , f_{ij} is the length of the triangle edge between C_i and C_j , and h_{ij} is the length of the dual edge connecting the circumcenters of C_i and C_j .

The numerical scheme is then obtained by applying a variational discretization in time, [6].

3 Numerical Results

On a small selection of test cases of fluid and geophysical fluid dynamics on an f-plane or the sphere, we show the performance of the variational integrators developed in [1,2]. We focus here on illustrating similarities and differences between the models and their variational discretizations.

Consider first the RSW scheme on both an f-plane and the sphere. We study the scheme's capability to conserve steady state solutions, cf. [1,5], and invariants such as mass, energy, potential vorticity and enstrophy. Figure 2 shows that for long term integrations, the total energy (kinetic + potential energy) is well preserved for simulations on a regular (left) and irregular (middle) f-plane mesh, but also rather well on the sphere (right).



Fig. 2. Relative errors in total energy for the RSW scheme over 1 year. Left and middle: isolated vortex solutions [1] on uniform, resp. non-uniform meshes (64^2 triangles) on an *f*-plane; right: TC 2 solutions [5] on the sphere (10242 Voronoi cells).

Note that mass and potential vorticity are preserved at machine precision for all cases. Although not by construction, potential enstrophy is well preserved too on both f-plane and the sphere: for 50 days run of TC 2 of [15] at 10^{-7} and for TC 5 at 10^{-3} . In general we notice that the solutions on the f-plane and on the sphere behave very similarly.

Consider further the convergence plots for the RSW scheme on a regular and irregular f-plane mesh (left) and on the sphere (right) of Fig. 3. The plots show the convergence of the numerical results after 1 day, resp. 12 days of simulations against the corresponding steady state solutions. On the *f*-plane, our



Fig. 3. Convergence of RSW scheme. Left: on the sphere for steady state solution (WTC2) after 12 days. Right: on an f-plane for steady state solutions after 1 day.

scheme shows at least 1st order convergence rates, while on the sphere, given the additional curvature, it reduces to the order of about 0.5.

Figure 4 shows the fluid depth after a simulation of 14 days for TC 2 (left) and a Rossby wave [5]. A comparison to literature confirms that these solutions are accurately represented by our RSW integrator.



Fig. 4. RSW scheme on the sphere. Left: Williamson test case 5 (flow over a mountain) after 14 days. Right: Rossby wave test case. Colorbars indicate fluid depth in [m]. (Color figure online)

Finally, Fig. 5 shows solutions of the cold bubble test case [3], i.e. a falling cold bubble in a warm environment. The left panel presents the solution of the anelastic model with a linearized buoyancy term, the right one the corresponding



Fig. 5. Potential temperature θ on regular meshes: comparison of results of the anelastic (left) and pseudo-incompressible schemes (right) for the falling cold air bubble with $\theta_{min}/\theta_{max} = 90 \text{ K}/300 \text{ K}$. Colorbar indicates $[\theta]$ in K.

solution for the pseudo-incompressible (PI) scheme applying a nonlinear buoyancy approximation. Our PI captures well the physical meaningful nonlinear effect that prevents the bubble from stretching [3,11], in contrast to the anelastic scheme. Matching well the results from literature, this confirms the accuracy of the variational schemes for the soundproof models.

4 Conclusions

We presented a variational discretization framework for geophysical flow models. This framework unifies the integrators for soundproof and compressible flow models developed in [1,2]. In particular, we could illustrate that the methodology of deriving discrete velocity fields as elements of discrete Lie algebras of the fluid models has many steps in common, while the discrete Lie groups that approximate the configuration space and the advection of either buoyancy or the fluid density of soundproof or compressible fluids, respectively, naturally differ. We illustrated on some selected numerical results simularities and differences between these variational integrators while confirming their excellent conservation properties.

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