Towards Structure Preserving Discretizations of Stochastic Rotating Shallow Water Equations on the Sphere

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joint work with:

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Motivation

Discrete variational principle

Variational integrator and Casimir dissipation for RSW

Numerical results for determinsitic schemes

Stochastic RSW model

Numerical results for stochastic schemes

Conclusions

Motivation

Overview: towards structure-preserving stochastic flow models

Structure preserving discretization:

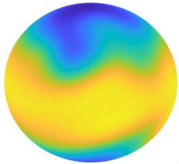
preservation of key structural properties

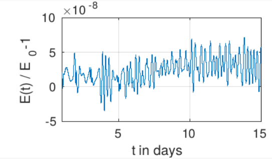
- Cohomology (deRham complex):
  $V_0(\mathbb{R}) \xrightarrow{\nabla} V_1(\mathbb{R}^3) \xrightarrow{\nabla\times} V_2(\mathbb{R}^3) \xrightarrow{\nabla\cdot} V_3(\mathbb{R})$
- Variational structure $\delta \int \ell = 0$
- Hamiltonian structure $\dot{\mathcal{F}} = \{\mathcal{F}, \mathcal{H}\}$

Why important?

- convergence to correct solutions
- correct energy transfer betw. scales
- correct statistical means

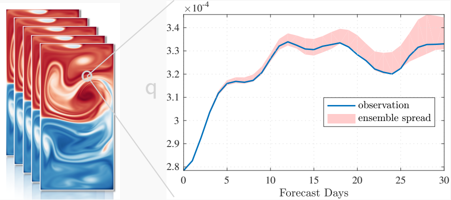
Example: Energy conservation





Stochastic modeling, UQ, DA:

to model uncertainty and include data



A reliable ensemble forecast of enstrophy q by the stochastic quasi-geostrophic scheme

Efficiency and scalability:

- Space and time parallelization
- Scalable augmented Lagrangian preconditioner
- Automated code generation (e.g Firedrake)

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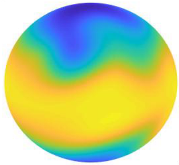

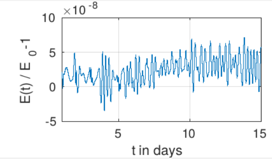

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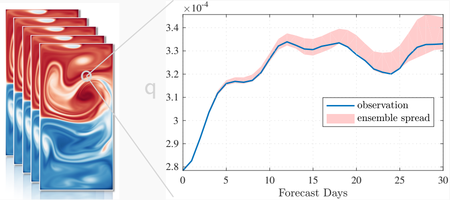

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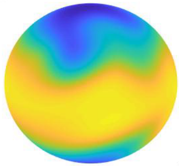

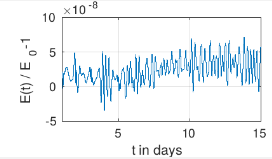

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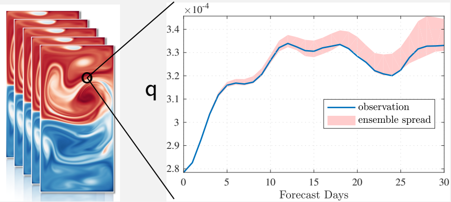

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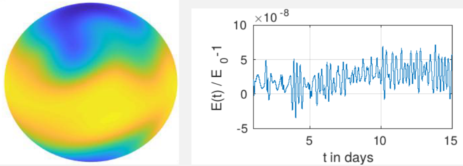

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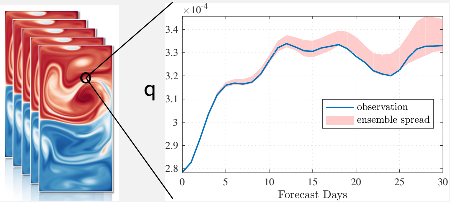

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Discrete variational principle

(Discrete) variational principle

Continuous variational Lagrangian method

For ℓ Lagrangian, u div-free velocity:

- variational principle: $\delta \int_0^T \ell(\mathrm{u}) dt = 0$ leads to (Holm et al. 98)

- Euler-Poincaré (EP) eqns: $\partial_t \frac{\delta \ell}{\delta \mathrm{u}} + \mathcal{L}_{\mathrm{u}} \frac{\delta \ell}{\delta \mathrm{u}} = -\mathrm{d}p$ with Lie derivative $\mathcal{L}$, pressure p

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$\frac{\delta \ell}{\delta \mathrm{u}} = \mathrm{u} \quad \rightarrow \quad \partial_t \mathrm{u} + \mathrm{u} \cdot \nabla \mathrm{u} = -\nabla p$

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- EP theory: $\frac{\delta}{\delta \mathrm{u}} \rightarrow \frac{\delta_d}{\delta \mathrm{u}_d}$, $\mathcal{L} \rightarrow \mathcal{L}^d, \ldots$

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Very general discretization method:
- for $\ell_d \rightarrow$ discrete structure preserving eqns. of motion
- currently FD-like matrix-vector eqns.

Variational integrator and Casimir dissipation for RSW

Overview: EP-theory for compressible fluids

METHOD: Step by step translation of Euler Poincaré theory

Continuous → Discrete

Continuous diffeomorphisms	Discrete diffeomorphisms
$\mathrm{Diff}(\mathcal{M}) \ni \varphi$	$\mathrm{D}(\mathbb{M}) \ni q$
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
$h \mapsto h \bullet \varphi = (h \circ \varphi) J\varphi$	$D \mapsto D \bullet q = \Omega^{-1} q^{\mathsf{T}} \Omega D$
Eulerian velocity and advected quantity	Disc. Eulerian veloc. and advec. quantity
$\mathrm{u} = \dot{\varphi} \circ \varphi^{-1},\;\; h = (h_0 \circ \varphi^{-1}) J\varphi^{-1}$	$A = \dot{q} q^{-1},\;\; D = \Omega^{-1} q^{-\mathsf{T}} \Omega D_0$
Euler-Poincaré principle	Euler-Poincaré-d'Alembert principle
$\delta \int_0^T \ell(\mathrm{u}, h) dt = 0, \delta \mathrm{u} = \partial_t \mathrm{v} + [\mathrm{v}, \mathrm{u}]$ $\delta h = -\operatorname{div}(h\mathrm{v})$	$\delta \int_0^T \ell(A, D) dt = 0, \delta A = \partial_t B + [B, A]$ $\delta D = -\Omega^{-1} B^{\mathsf{T}} \Omega D, \quad A, B \in \mathcal{S} \cap \mathcal{R}$

Table 1: Continuous and discrete objects for compressible discretizations. The divergence is denoted by div and the Jacobian by J.

Variational discretization of rotating shallow water (RSW)

1) Discrete diffeomorphism groups

- $\mathsf{D}(\mathbb{M}) = \left\{ q \in \mathsf{GL}(N)^+ \mid q \cdot 1 = 1 \right\}$,
  - with constant discrete function $1 = (1, \ldots, 1)^\mathsf{T}$
  - $q \cdot 1 = 1$ encodes, at the discrete level, the fact that constant functions are preserved under composition by a diffeomorphism

Action of group on discrete functions

$$\begin{tikzcd}
f \in \mathcal{F}(\mathcal{M}) \arrow[r, "\mathrm{Diff}(\mathcal{M})"] \arrow[d, "\text{Discretization}"] & f \circ \varphi^{-1} \in \mathcal{F}(\mathcal{M}) \arrow[d, "\text{Discretization}"] \\
F \in \mathbb{R}^N \arrow[r, "\mathsf{D}(\mathbb{M})"] & q \cdot F = F \circ q^{-1} \in \mathbb{R}^N
\end{tikzcd}$$

2a) Discrete Lie algebras

By taking the derivative of continuous and discrete actions at the identity, we get $\frac{d}{dt}\Big|_{t=0} f \circ \varphi_t^{-1} = -\mathrm{d}f \cdot \mathrm{u}$ and $\frac{d}{dt}\Big|_{t=0} F \circ q_t^{-1} = AF$, where $\frac{d}{dt}\Big|_{t=0} \varphi_t = \mathrm{u}$ and $\frac{d}{dt}\Big|_{t=0} q_t = A$.

$\Rightarrow$ AF is discretization of (minus) the derivative of f in direction u

Lie algebras:

- $\mathfrak{d}(\mathbb{M}) = \{A \in \mathrm{Mat}(N) \mid A \cdot 1 = 0\}$,

Not all $A \in \mathfrak{d}(\mathbb{M})$ can be interpreted as discrete vector fields

$\Rightarrow$ *nonholonomic constraints* are required for the variational principle

2b) Nonholonomic constaints

- fluxes nonzero only between neighboring cells $\Rightarrow$
  linear constraint $\mathcal{S} = \big\{A \in \mathfrak{d}(\mathbb{M}) \mid A_{ij} = 0,\ \forall\, j \notin N(i)\big\}$
  $N(i)$ set of indices of cells adjacent to cell i.

- additional constraint, $\Omega_{ii}A_{ij} = -\Omega_{jj}A_{ji}$, for all $j \neq i \Rightarrow$
  linear constraint $\mathcal{R} = \big\{A \in \mathfrak{d}(\mathbb{M}) \mid A^{\mathsf{T}}\Omega + \Omega A \text{ is diagonal}\big\}$.

These nonholonomic constraints are taken into account by using *Euler–Poincaré–d'Alembert principle*

2c) Discrete vector fields

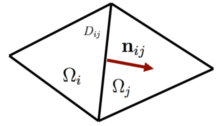
Subject to these nonholonomic constraints, matrix A approximates vector field u (convergence proof in Bauer & Gay-Balmaz (2019)):

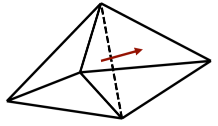
- matrix elements of $A \in \mathcal{S} \cap \mathcal{R}$ satisfy

$$A_{ij} \simeq -\frac{1}{2\Omega_{ii}} \int_{D_{ij}} (\mathrm{u} \cdot \mathrm{n}_{ij}) dS, \quad A_{ii} \simeq \frac{1}{2\Omega_{ii}} \int_{C_i} (\operatorname{div} \mathrm{u}) dx$$

,

for all $j \in N(i)$, $j \neq i$, with D_{ij} the hyperface common to cells C_i and C_j and n_{ij} is the normal vector on D_{ij} pointing from C_i to C_j





In Bauer & Gay-Balmaz (2019) we proved convergence of the velocity field.

3) Discrete advected quantities

Definition of action of discrete group elements on advected quantities:

- for discrete fluid density D:

$$D \mapsto D \bullet q = \Omega^{-1} q^{\mathsf{T}} \Omega D$$

  because action of discrete density is dual to action on discrete functions: $\langle D \bullet q, F \rangle = \langle D, F \circ q^{-1} \rangle$ for all $F \in \mathbb{R}^N$, wrt to L2 pairing

4) Discrete Euler–Poincaré–d'Alembert (EPA) principle

$$\delta \int_0^T \ell_d(A, D) dt = 0$$

with constraint variations $\delta A = \partial_t B + [B, A]$, $B(0) = B(T) = 0$, and

- $\delta D = -D \bullet B$, with $A, B \in \mathcal{S} \cap \mathcal{R}$,

Discrete EPA principle yields

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

with projection P associated to nonholonomic constraints; and with discrete continuity equation $\frac{d}{dt} D + D \bullet A = 0$.

Example: compressible RSW equations

- Define discrete Lagrangian

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

as approximation of continuous Lagrangian of RSW

$$\ell(\mathrm{u}, \rho) = \int_M \left[\frac{1}{2}\rho\, \mathrm{u}^\flat \cdot \mathrm{u} + \rho\, \mathrm{R}^\flat \cdot \mathrm{u} - \frac{1}{2} g (h + B)^2\right] dx,$$

- Define discrete pairings to calculate discrete functional derivatives

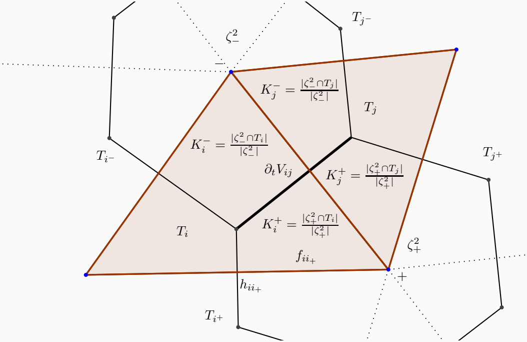
$$\langle\langle K, A\rangle\rangle := \mathrm{Tr}\left(K^\mathsf{T} \Omega A\right), K \in \Omega^1_d(\mathbb{M}), \langle F, G\rangle := F^\mathsf{T} \Omega G = \sum_{i=1}^{N} F_i \Omega_i G_i,\ F, G \in \mathbb{R}^N$$

- Calculate discrete functional derivatives wrt. to these pairings

$$\frac{\delta \ell}{\delta A_{ij}} = D_i (A^\flat_{ij} + R^\flat_{ij}) \quad \text{and} \quad \frac{\delta \ell}{\delta D_i} = \frac{1}{2}\sum_j A^\flat_{ij} A_{ij} + \sum_j R^\flat_{ij} A_{ij} - g(D_i + B_i)$$

- Variational scheme follows from discrete EPA principle

For 2D triangular mesh with certain choice of $\flat$ and $[,]$ according to Pavlov et al 2010



Semi-discrete RSW equations on triangular grid:

$$\left\{\begin{aligned}
&\overline{D}_{ij}\frac{d}{dt}A^\flat_{ij} + \omega_+\left(K_i^+\overline{D}_{ji_+}A_{ii_+} + K_j^+\overline{D}_{ij_+}A_{jj_+}\right) - \omega_-\left(K_i^-\overline{D}_{ji_-}A_{ii_-} + K_j^-\overline{D}_{ij_-}A_{jj_-}\right)\\
&\qquad\qquad +\overline{D}_{ij}\frac{1}{2}\left(A^\flat_{ii_-}A_{ii_-} + A^\flat_{ii_+}A_{ii_+} + A^\flat_{ij}A_{ij} - A^\flat_{ji}A_{ji} - A^\flat_{jj_-}A_{jj_-} - A^\flat_{jj_+}A_{jj_+}\right)\\
&\qquad\qquad +\overline{D}_{ij}g\left((D_i + B_i) - (D_j + B_j)\right) = 0\\
&\frac{d}{dt}D_i = A_{ii_-}D_{i_-} + A_{ii_+}D_{i_+} + A_{ij}D_j - A_{ii}D_i,
\end{aligned}\right.$$

with $\overline{D}_{ij} := \frac{1}{2}(D_i + D_j)$ and $\omega_\pm := \sum_{\zeta^1_{mn}\in\partial\zeta_\pm}(A^\flat_{mn} + R^\flat_{mn})$ the discrete absolute vorticity at node $\pm$

Variational time discretization

Time integration (structure preserving)

1. D as advected quantity are updated by discrete Cayley transform
2. Momentum equation is updated by Crank-Nicolson type time scheme

This gives variational discretizations for RSW equations in both space and time

Casimir dissipation for RSW

Let $\ell\colon \mathfrak{d}(\mathrm{M}) \times \mathsf{D}_d^{en}(\mathrm{M}) \to \mathrm{R}$ be a semi-discrete Lagrangian and $C\colon \mathfrak{d}(\mathrm{M}) \times \mathsf{D}_d^{en}(\mathrm{M}) \to \mathrm{R}$ be a semi-discretized approximation of a Casimir. Let $\gamma\colon \mathfrak{d}(\mathrm{M}) \times \mathfrak{d}(\mathrm{M}) \to \mathrm{R}$ be a positive, symmetric bilinear form.

Consider discrete dissipative variational principle:

$$\delta \int_0^T \ell(A, D)\mathrm{d}t + \theta \int_0^T \gamma\left(\left[\frac{\delta C}{\delta M}, A\right], [A, B]\right) \mathrm{d}t = 0 \quad \text{for} \quad \begin{cases} \delta A = \partial_t B + [B, A] \\ \delta D = -\Omega^{-1} B^\top \Omega D \end{cases} \tag{1}$$

with $B \in \mathcal{R}$ and $B(0) = B(T) = 0$. M is discrete momentum.

Theorem (Discrete dissipative variational equations)

For a semi-discrete Lagrangian $\ell(A, D)$, *the curves* $A(t), D(t)$ *are critical for the variational principle of Eq.* (1) *if and only if they satisfy*

$$P\left(\frac{d}{dt}\frac{\delta \ell}{\delta A} + \mathcal{L}_A\left(\frac{\delta \ell}{\delta A}\right) - \theta \mathcal{L}_A\left(D\left[\frac{\delta C}{\delta M}, A\right]^{\flat}\right) + D\frac{\delta \ell}{\delta D}^{\top}\right)_{ij} = 0, \tag{2}$$

where $\langle \mathcal{L}_A M, B\rangle_1 = \langle M, [A, B]\rangle_1$.

Proof in *Brecht, R., Bauer, W., Bihlo, A., Gay-Balmaz, F. and MacLachlan, S. [2021], Selective decay for the rotating shallow-water equations with a structure-preserving discretization, Physics of Fluids,* 33, *116604.*

NOTE:

- for the resulting semi-discrete scheme, the energy is conserved.
- dissipation of Casimir “only” shown numerically

Casimir dissipative RSW scheme

In terms of velocity V and water depth D, and for $\theta > 0$, the Casimir dissipative momentum equation is

$$\partial_t V_{ij} = -\mathsf{Adv}(V, D)_{ij} - \mathsf{K}(V)_{ij} - \mathsf{G}(D)_{ij} + \theta \mathsf{L}(V, D, \frac{\delta C}{\delta M})_{ij}, \tag{3}$$

where

$$P\left(\mathcal{L}_A\left(D\left[\frac{\delta C}{\delta M}, A\right]^\flat\right)\right)_{ij} =: \mathsf{L}(V, D, \frac{\delta C}{\delta M})_{ij}.$$

- Black terms in (3) correspond to original scheme (in terms of V and D)
- Orange term in (3) is Casimir dissipation term
- $P, \mathcal{L}_A$ operators derived for original scheme
- Problem: because $[A, B] \in [\mathcal{R}, \mathcal{R}]$, for $A, B \in \mathcal{R}$ and $[\mathcal{R}, \mathcal{R}] \neq \mathcal{R}$, Pavlov et al 2009 method does not work here!

Idea in Brecht at al 2021: Vector calculus approximation of $\left[\frac{\delta C}{\delta M}, A\right]$ such that it is in $\mathcal{R}$

Casimir C of interest here: Enstrophy

Continuous enstrophy Casimir $C(m,h) = \frac{1}{2}\int_{\mathcal{M}} h\, q(\mathrm{m},h)^2 \mathrm{d}\sigma$

Discrete enstrophy Casimir:

$$\mathcal{C}(M,D) = \frac{1}{2}\sum_{\zeta} D_\zeta \Big(q(M,D)_\zeta\Big)^2 |\zeta|, \qquad q(M,D)_\zeta = \frac{(\text{Curl } V) + f}{D_\zeta},\ D_\zeta = \sum_{T_i\cap\zeta\neq\emptyset} \frac{|T_i\cap\zeta|}{|\zeta|} D_i,$$

where $M = \frac{\delta\ell}{\delta A}$, f is the Coriolis parameter, and dual cell ζ

Discrete variational derivative:

$$\frac{\delta\mathcal{C}}{\delta M}_{ij} = \frac{q_{\zeta_+} - q_{\zeta_-}}{\Omega_{ii} h_{ij}} = -\frac{|e_{ij}|}{2\Omega_{ii}}\Big(2\frac{q_{\zeta_-} - q_{\zeta_+}}{|e_{ij}|}\frac{1}{h_{ij}}\Big) = -\frac{|e_{ij}|}{2\Omega_{ii}}\frac{2 \text{ Grad}_t\ q}{h_{ij}}.$$

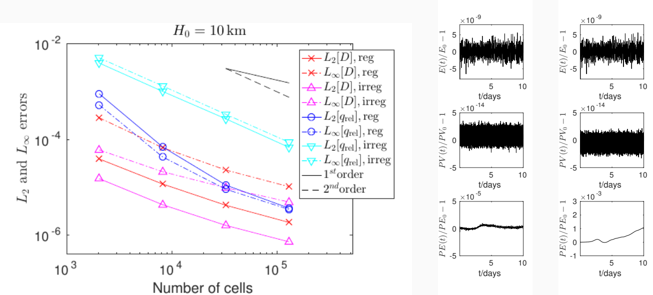
NOTE:

- approximation of enstrophy Casimir is not a Casimir of the discrete system
- we cannot directly prove that enstrophy is dissipated
- numerical results demonstrate that scheme dissipates enstrophy

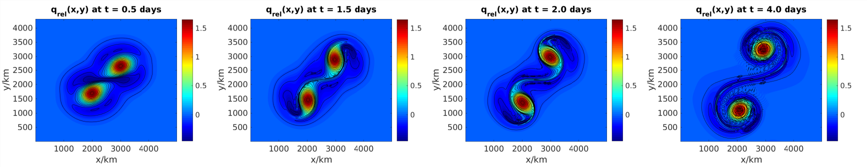
Numerical results for determinsitic schemes

Results for variational discretization of RSW equations (Bauer & Gay-Balmaz 2019)

- Convergence of numerical to analytic (steady state) solution
- Conservation of mass, total energy, PV; NO enstrophy conservation (accumulation at small scales)
- Correct representation of nonlinear dynamics



For regular and nonuniform (irreg) meshes; Left: convergence of numerical to steady state solution. Right: Diagnostics for E, potential vorticity PV and enstrophy PE



Time evolution of the relative vorticity $q_{\mathrm{rel}}(x, y)$: dual vortices interaction

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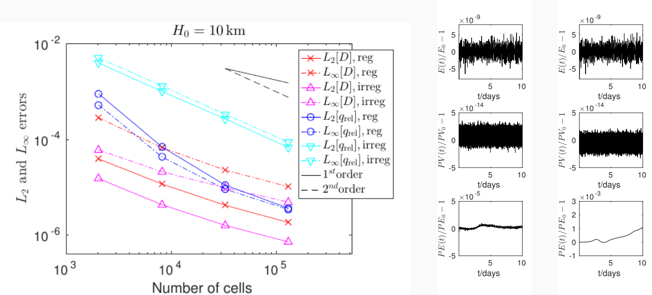

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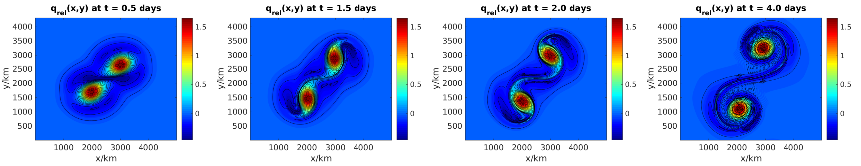

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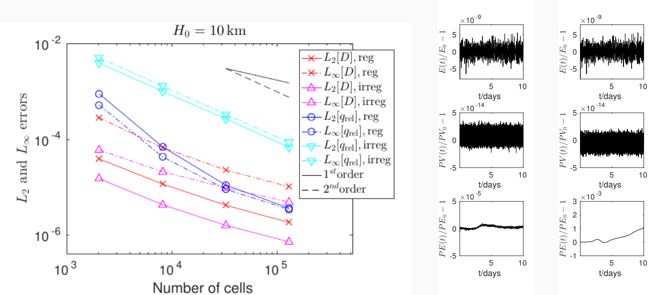

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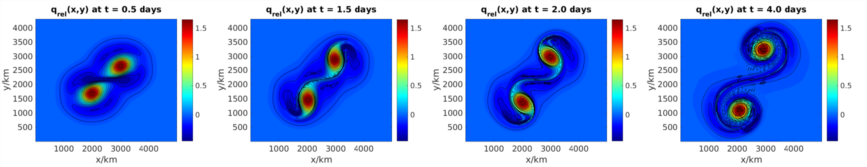

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Results for variational discretization of RSW equations

- Variational RSW (Var-RSW) scheme (Bauer etal. 2019, Brecht etal. 2019) with no dissipation (ND)
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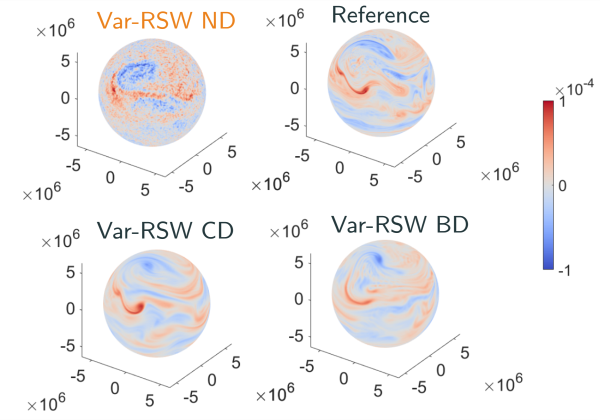
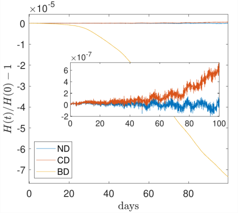
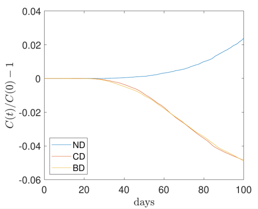
- Reference obtained with compatible FEM method using SUPG dissipation







Comparison of relative vorticity fields: flow over mountain after 100 days

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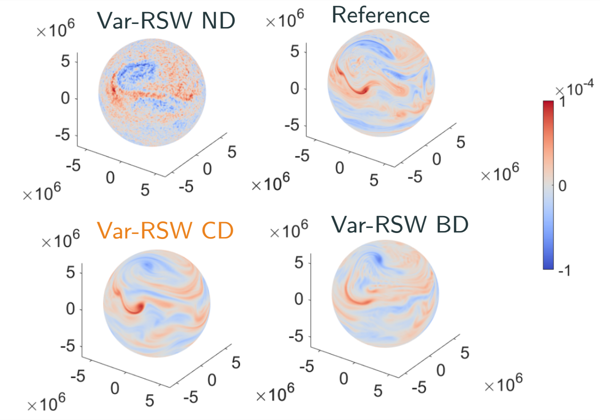

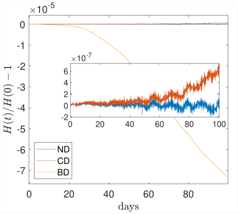

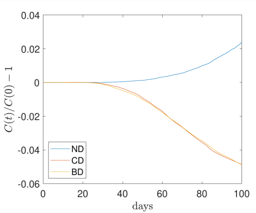

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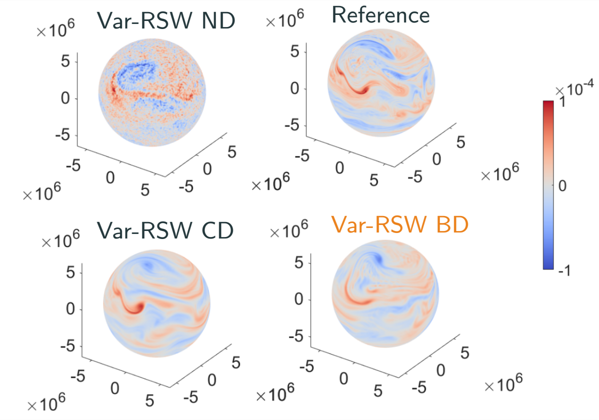

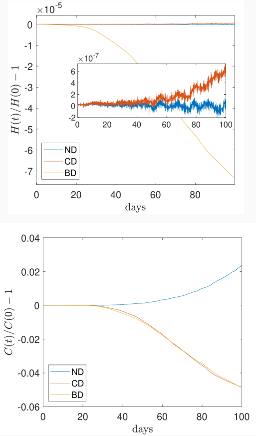

Comparison of relative vorticity fields: flow over mountain after 100 days

Stochastic RSW model

Stochastic structure-preserving RSW model

Assumption: fast-slow decomposition of velocity:

$$\mathrm{d}\boldsymbol{X}_t = \boldsymbol{w}(\boldsymbol{X}_t, t)\,\mathrm{d}t + \boldsymbol{\sigma}(\boldsymbol{X}_t, t)\,\mathrm{d}\boldsymbol{B}_t,$$

$\boldsymbol{X}$ Lagrangian displacement, $\boldsymbol{w}$ large-scale velocity (spatially and temporally correlated), $\boldsymbol{\sigma}\mathrm{d}\boldsymbol{B}_t$ highly oscillating unresolved component (correlated in space)

Derivation of consistent stochastic flow models:
i) Holm 15 (SALT): $\delta \int \left(\ell(\mathrm{u}, q)dt + \langle p, dq + \mathcal{L}_{dx_t} q\rangle_{L^2}\right) = 0$, $\mathcal{L}$ Lie derivative of advected quantity q, p Lagrange multiplier
ii) Memin 14 (Location Uncertainty (LU)): stochastic Reynolds transport theorem

Stochastic RSW-LU:

$$\mathrm{d}_t\boldsymbol{u} = \Big(-\boldsymbol{u}\cdot\boldsymbol{\nabla}\,\boldsymbol{u} - \boldsymbol{f}\times\boldsymbol{u} - g\boldsymbol{\nabla}\eta\Big)\,\mathrm{d}t + \Big(\frac{1}{2}\,\boldsymbol{\nabla}\cdot\,\boldsymbol{\nabla}\cdot(\boldsymbol{a}\boldsymbol{u})\,\mathrm{d}t - \boldsymbol{\sigma}\mathrm{d}\boldsymbol{B}_t\cdot\boldsymbol{\nabla}\,\boldsymbol{u}\Big),$$

$$\mathrm{d}_t h = -\,\boldsymbol{\nabla}\cdot\,(\boldsymbol{u}h)\,\mathrm{d}t + \Big(\frac{1}{2}\,\boldsymbol{\nabla}\cdot\,\boldsymbol{\nabla}\cdot(\boldsymbol{a}h)\,\mathrm{d}t - \boldsymbol{\sigma}\mathrm{d}\boldsymbol{B}_t\cdot\boldsymbol{\nabla}\,h\Big).$$

with variance (matrix) $\boldsymbol{a}$ measuring the strength of noise

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Structure-preserving discretization of RSW-LU (Brecht et al. 2021)

- Use variational RSW scheme for deterministic parts (Bauer et al. 2019)

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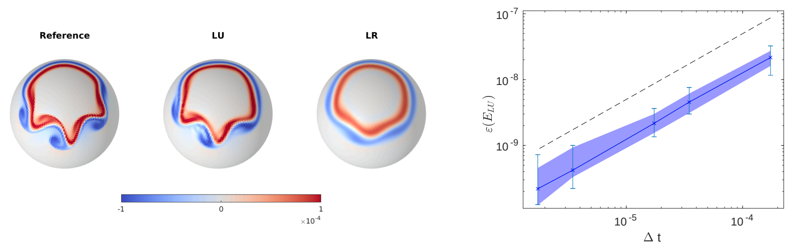
Structure-preserving discretization of RSW-LU (Brecht et al. 2021)

- Use variational RSW scheme for deterministic parts (Bauer et al. 2019)
- Approximate stochastic terms with standard finite difference operators

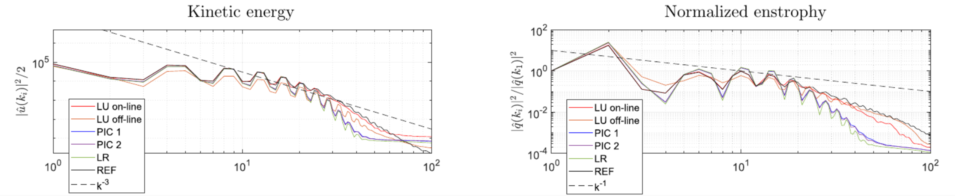
Numerical results for stochastic schemes

Results for structure-preserving stochastic RSW scheme (Brecht etal. 2021)

- Stochastic RSW-LU: each realization (ensemble member) preserves global energy
- Discretization is energy preserving (in space): noise balanced by dissipation terms
- Spectra of LU at small scales closer to REF as deterministic PIC 1/2



Large scales better represented by stochastic (LU) rather deterministic (LR) scheme, energy (in space) of each ensemble member preserved ($\approx 1^{st}$ order convergence)



Spectra of kinetic energy and enstrophy after 5 days

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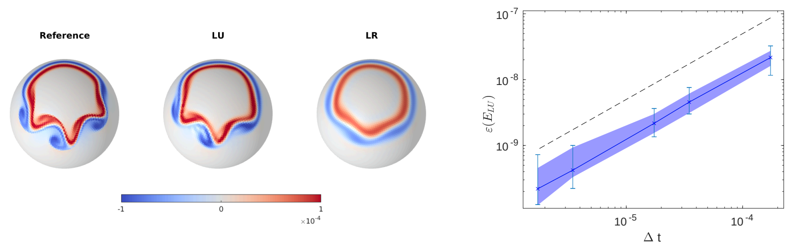

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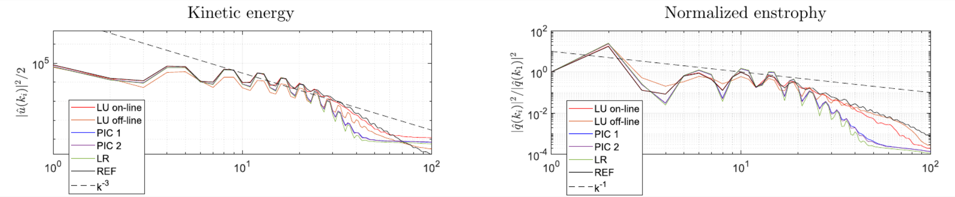

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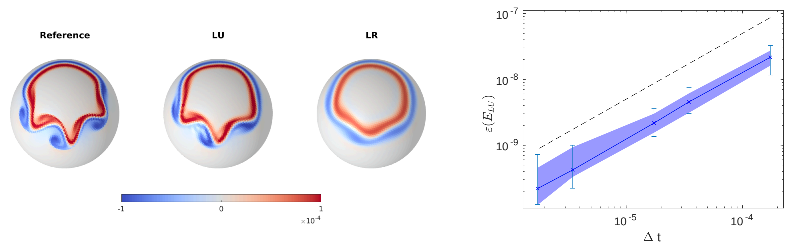

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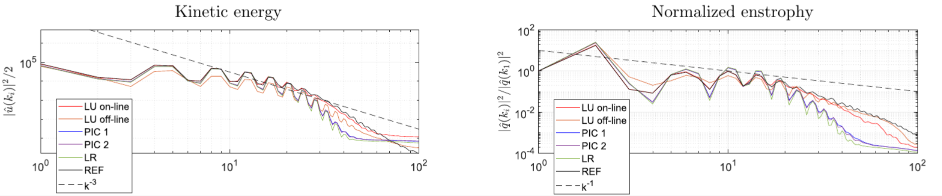
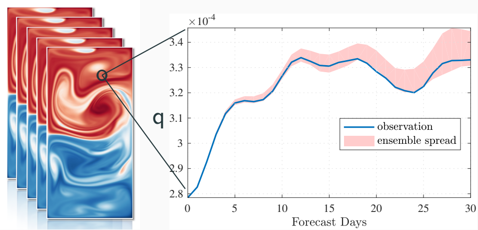


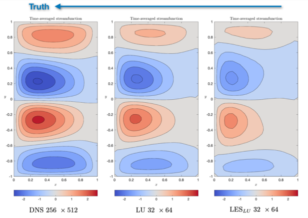
Spectra of kinetic energy and enstrophy after 5 days

Results for ensemble predictions (for QG and RSW equations)

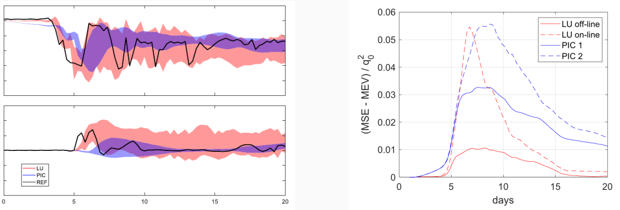
- More reliable ensemble spread with LU than deterministic perturbed initial conditions (PIC)
- LU better captures statistics than PIC
- NOTE: reliable spread important for data assimilation (DA)



Bauer etal 2020: reliable ensemble forecast of q of quasi-geostrophic LU-model



LU captures well stationary moments



Brecht etal. 2021: Left: ensemble spread (at 2 random points) of stochastic LU and det. PIC schemes for RSW on sphere. Right Error measure

Conclusions

Summary/Outlook

- We introduced (spatially) energy conserving stochastic RSW scheme (LU-RSW)
- Stochastic terms trigger large scale flow pattern even in low resolution runs;

  Reason: spectra of low-resolution LU-RSW exhibits sufficient small scales
- Ensemble spread more accurate than by a comparable LES scheme
- Statistics more accurate than by a comparable LES scheme

Outlook:

- Use Casimir dissipation instead of bilaplacian in stochastic LU-RSW
- Consistent stochastic model for data assimilation

Outlook: consistent stochastic models and data assimilation (DA)

Research goals:

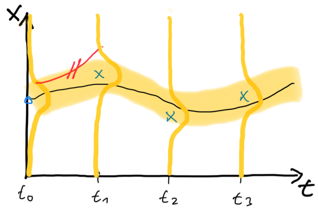
- Derive more complex stochastic flow models and schemes (e.g. 3D Euler)
- Use neural networks for noise parametrizations
- Develop consistent (structure-preserving) DA

Issue with standard methods (e.g. particle filter): localization techniques cut off correlations of not near data points, this usually destroys:

- geophysical flow balances (from balancing leading order forces)
- conservation of global invariants (from symmetries according to Noether)

Ideas for consistent DA:

- Preservation of balances: take into account geophysical balances when estimating σ
- Conservation of invariants: guarantee that covariance matrix after cutoff still preserves symmetries



DA: single realization, ensemble, data, cut off correlation

Literature

Structure-preserving discretizations of deterministic PDEs

- Brecht, R., Bauer, W., Bihlo, A., Gay-Balmaz, F. and MacLachlan, S. [2021], Selective decay for the rotating shallow-water equations with a structure-preserving discretization, *Physics of Fluids*, **33**, 116604.
- Brecht, R., Bauer, W., Bihlo, A., Gay-Balmaz, F. and MacLachlan, S. [2019], Variational integrator for the rotating shallow-water equations on the sphere, *Q. J. Royal Met. Soc.*, **145**, 1070-1088.
- Bauer, W. and Gay-Balmaz, F. [2019], Variational discretization framework for geophysical flow models, *Springer LNCS proceedings*: GSI 2019.
- Bauer, W. and Gay-Balmaz, F. [2019], Towards a variational discretization of compressible fluids: the rotating shallow water equations, *J. Comput. Dyn.*, **6**, 1–37.
- Bauer, W. and Gay-Balmaz, F. [2019], Variational integrators for anelastic and pseudo-incompressible flows, *J. Geom. Mech.*, **11**, 511-537.

Stochastic flow models and ensemble prediction

- Brecht, R., Li, L., Bauer, W. and Memin, E. [2021], Rotating shallow water flow under location uncertainty with a structure-preserving discretization, *Journal of Advances in Modeling Earth Systems*, **13**, e2021MS002492.
- Bauer, W., Chandramouli, P., Li, L. and Memin, E [2020], Stochastic representation of mesoscale eddy effects in coarse-resolution barotropic models, *Ocean Modelling*, **151**, 101646.
- Bauer, W., Chandramouli, P., Chapron, B., Li, L. and Memin, E. [2020], Deciphering the role of small-scale inhomogeneity on geophysical flow structuration: a stochastic approach, *Journal of Physical Oceanography*, **50**, 983–1003.

Thanks!

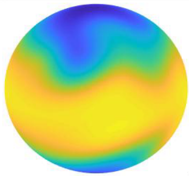
Additional slides!

Motivation: applications in Mathematics of Planet Earth

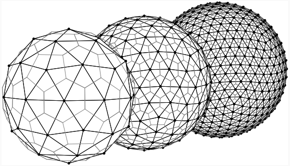
Geophysical Fluid Dynamics (GFD): Study of atmospheric and oceanic flows on rotating Earth

Some challenges:

- multiscale phenomena from meters (clouds) to 1000's of kilometers (large scale flow)
- integration times from hours (weather) to 1000's of years (climate)
- spherical geometry → nonregular meshes
- numerical algorithms:
  - efficient solvers
  - accurate and consistent
  - structure preserving



flow over mountain



E.g. Icosahedral meshes $\mathbb{M}$ with 80, 320, and 1280 cells

Various discretization methods

For PDEs, there is no single “best” numerical method for all needs!

State-of-the-art discretization method in GFD (for operational use):

	struct-preserv	consistency	efficiency	flexible, higher
DEC Discrete Exterior Calculus	✓	✗	✓	✗
FEEC Finite Element Exterior Calculus	✓	✓	✗	✓

✓: there is a way forward; ✗: no (satisfying) solution found yet

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My research activities (fill in ✓!) guided by question: How can geometric insights contribute to numerical modelling?

1. Variational Lagrangian DEC method (Finite Difference (FD))
2. Structure-preserving schemes in stochastic fluid dynamics
3. Hamiltonian FEEC method
4. split Hamiltonian FE(EC), split equations of GFD

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Remark: following mathematical methods and numerical algorithms are

Thanks for your attention!

Additional slides!

(1) Variational principles for structure-preserving discretizations in GFD

Hamilton's principle for ODEs

For Lagrangian $L : \mathbb{R}^N \times \mathbb{R}^N \to \mathbb{R}$, we search extremum

$$\delta \mathcal{S} = \delta \int_0^T L(\mathrm{q}(t), \dot{\mathrm{q}}(t))dt = 0$$

$\mathrm{q} = \{q_1, \ldots, q_N\}$ generalized coordinates; small variations $\delta \mathrm{q}$ vanishing at endpoints t_1 and t_2

Variations of L and integration by parts:

$$0 = \delta \mathcal{S} = \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial \mathrm{q}} \delta \mathrm{q} + \frac{\partial L}{\partial \dot{\mathrm{q}}} \delta \dot{\mathrm{q}} \right) dt$$

$$= \cancel{\left[\delta \mathrm{q} \frac{\partial L}{\partial \dot{\mathrm{q}}} \right]_{t_1}^{t_2}} + \int_{t_1}^{t_2} \delta \mathrm{q} \left(\frac{\partial L}{\partial \mathrm{q}} - \frac{d}{dt} \frac{\partial L}{\partial \dot{\mathrm{q}}} \right) dt$$

Euler-Lagrange equations

$$\frac{\partial L}{\partial \mathrm{q}} - \frac{d}{dt} \frac{\partial L}{\partial \dot{\mathrm{q}}} = 0$$

$\Rightarrow$ equations of motion for any L

Hamilton's principle for (incomp.) fluids

For $L_{\Theta_0}(\varphi_t, \dot{\varphi}_t) : TDiff(\mathcal{D}) \to \mathbb{R}$, we search extremum

$$\delta S = \delta \int_0^T L_{\Theta_0}(\varphi_t, \dot{\varphi}_t)dt = 0$$

$G = Diff(M)$ Lie group of vol-preserv. diffeomorphisms; flow map $\varphi_t : X \in \mathcal{D}$ at $t = 0$ to $x = \varphi_t(X)$ at t

Euler (spatial) representation: For spatial Lagrangian $\ell(\mathrm{u}, \theta) : \mathfrak{X}(\mathcal{D}) \times \mathcal{F}(\mathcal{D}) \to \mathbb{R}$, we search extremum

$$\delta \int_0^T \ell(\mathrm{u}, \theta)dt = 0, \delta \mathrm{u} = \partial_t \mathrm{v} + [\mathrm{v}, \mathrm{u}], \delta \theta = -\mathrm{v} \cdot \nabla \theta$$

$\mathrm{u}(x, t)$ Eulerian velocity field in Lie algebra $\mathfrak{X}$, $\mathrm{v}(x, t) \in \mathfrak{X}(\mathcal{D})$ is div-free arbitrary vector field on $\mathcal{D}$, $\theta(x, t) \in \mathcal{F}(\mathcal{D})$ is advected potential temperature

Euler-Poincaré equations

$$\partial_t \frac{\delta \ell}{\delta \mathrm{u}} + \mathrm{u} \cdot \nabla \frac{\delta \ell}{\delta \mathrm{u}} + \nabla \mathrm{u}^{\mathsf{T}} \cdot \frac{\delta \ell}{\delta \mathrm{u}} + \frac{\delta \ell}{\delta \theta} \nabla \theta = -\nabla p, \; \partial_t \theta + \mathrm{u} \cdot \nabla \theta = 0,$$

in which p is pressure and ∇ is covariant derivative or gradient

(1) Variational principles for structure-preserving discretizations in GFD

Discrete Hamilton's principle for fluids

Step by step translation of EP

Continuous → Discrete

Step 1: Continuous diffeomorphisms	Discrete diffeomorphisms
$\mathrm{Diff}(M) \ni \varphi$	$\mathrm{D}(\mathbb{M}) \ni q$
Step 2: Group action on functions	Group action on discrete functions
$f \mapsto f \circ \varphi^{-1}$	$F \mapsto F \circ q^{-1} = qF$
Step 3: Eulerian velocity & temp.	Discrete velocity and disc. temp.
$\mathrm{u} = \dot{\varphi} \circ \varphi^{-1}, \;\; \theta = \Theta_0 \circ \varphi^{-1}$	$A = \dot{q}q^{-1}, \;\; \Theta = q\Theta_0$
Step 4: Euler-Poincaré principle	Euler-Poincaré-d'Alembert principle
$\delta \int_0^T \ell(\mathrm{u}, \theta) dt = 0,$ $\delta \mathrm{u} = \partial_t \mathrm{v} + [\mathrm{v}, \mathrm{u}], \;\; \delta\theta = -\mathrm{d}\theta \cdot \mathrm{v}$	$\delta \int_0^T \ell(A, \Theta) dt = 0,$ $\delta A = \partial_t B + [B, A], \;\; \delta\Theta = B\Theta$ constraint: $A, B \in \mathcal{S}$

(1) Variational principles for structure-preserving discretizations in GFD

Discrete Hamilton's principle for fluids

Step by step translation of EP

Continuous → Discrete

Step 1: Continuous diffeomorphisms	Discrete diffeomorphisms
$\mathrm{Diff}(M) \ni \varphi$	$\mathrm{D}(\mathbb{M}) \ni q$
Step 2: Group action on functions	Group action on discrete functions
$f \mapsto f \circ \varphi$	$F \mapsto q^{-1} F = F \circ q$
Step 3: Eulerian velocity and depth	Eulerian discrete velocity and discrete depth
$\mathrm{u} = \dot{\varphi} \circ \varphi^{-1}$, $h = (h_0 \circ \varphi^{-1}) J\varphi^{-1}$	$A = \dot{q} q^{-1}$, $D = \Omega^{-1} q^{-\mathsf{T}} \Omega D_0$
Step 4: Group action on densities	Group action on discrete densities
$h \mapsto h \bullet \varphi = (h \circ \varphi) J\varphi$	$D \mapsto D \bullet q = \Omega^{-1} q^{\mathsf{T}} \Omega D$
Step 5: Euler-Poincaré principle	Euler-Poincaré-d'Alembert principle
$\delta \int_0^T \ell(\mathrm{u}, h) dt = 0$, $\delta \mathrm{u} = \partial_t \mathrm{v} + [\mathrm{v}, \mathrm{u}]$, $\delta h = -\operatorname{div}(h\mathrm{v})$	$\delta \int_0^T \ell(A, D) dt = 0$, $\delta A = \partial_t B + [B, A]$, $\delta D = -\Omega^{-1} B^{\mathsf{T}} \Omega D$ constraint: $A, B \in \mathcal{S} \cap \mathcal{R}$