Structure-preserving models of geophysical fluids

Chris Eldred, Thomas Dubos, Daniel Le Roux and Francois Gay-Balmaz

April 30th, 2019

Outline of Talk

1. Motivation and Overview
2. Reversible (Entropy-Conserving) Dynamics
3. Irreversible (Entropy-Generating) Dynamics
4. Summary and Outlook

1 Motivation and Overview

2 Reversible (Entropy-Conserving) Dynamics

3 Irreversible (Entropy-Generating) Dynamics

4 Summary and Outlook

What makes geophysical fluids hard to model?

1. Not solving **arbitrary PDEs**: building model of a **physical system** (no analytic solutions)
2. Multiscale, (usually) multiphase, multicomponent fluids
3. Limited computer power → limited resolution → **parameterizations**
4. Differential equations → **algebraic equations**
5. **Do algebraic solutions have the same properties as the differential (true) solutions?**

(Incomplete) List of Desirable Model Properties

Realistic Simulations

Control Over Approximations
- -Non-traditional/Deep
- -Non-Spherical Geopotential
- -Arbitrary Equations of State

Linear Modes
- -No Spurious Stationary Modes
- -Good Dispersion Relationship
- -No Spurious Branches of Waves
- -No Inertial Modes

Accuracy
- -Taylor Series Sense
- -Convergence to Reference Solutions

Balanced Dynamics
- -No Spurious Vorticity Generation
- -Hydrostatic Balance
- -Steady Geostrophic Modes

Conservation
- -Mass
- -Energy
- -Entropy/Potential Temperature
- -Moisture/Tracers

Compatible Advection
- -Thermodynamic Variables
- -Tracers/Moisture

Efficiency
- -Strong/Weak Scalability
- -Time to Solution

Stability
- -No Hollingsworth Instability
- -Nonlinear Stability

Generality
- -Reversible Dynamics
- -Irreversible Dynamics

Other
- -Geometric Flexibility
- -Inactive Regions

How can we obtain this (large) set of properties?

A General Approach to Obtain These Properties

A systematic, general approach to structure-preserving discretization is:

1. Start with a bracket formulation:
$$\frac{\partial \mathbf{x}}{\partial t} = \mathbb{J}(\mathbf{x})\frac{\delta \mathcal{H}}{\delta \mathbf{x}}(\mathbf{x}) + \mathbb{M}(\mathbf{x})\frac{\delta \mathcal{S}}{\delta \mathbf{x}}(\mathbf{x})$$
2. Discretize space with a mimetic discretization scheme $\rightarrow$ metriplectic system of ODEs
$$\frac{\partial \mathbf{x}}{\partial t} = \mathbf{J}(\mathbf{x})\nabla\mathcal{H}(\mathbf{x}) + \mathbf{M}(\mathbf{x})\nabla\mathcal{S}(\mathbf{x})$$
3. Discretize time with an energy-conserving metriplectic integrator ex. discrete gradient method

$$\frac{\mathbf{x}^{n+1} - \mathbf{x}^n}{\Delta t} = \widetilde{\mathbf{J}}(\mathbf{x}^{n+1}, \mathbf{x}^n)\bar{\nabla}\mathcal{H}(\mathbf{x}^{n+1}, \mathbf{x}^n) + \widetilde{\mathbf{M}}(\mathbf{x}^{n+1}, \mathbf{x}^n)\bar{\nabla}\mathcal{S}(\mathbf{x}^{n+1}, \mathbf{x}^n)$$

This gives most of the properties $\rightarrow$ choose specific mimetic spatial and temporal discretizations to get the rest

What properties do we get? What remains?

Realistic Simulations

Control Over Approximations
- -Non-traditional/Deep
- -Non-Spherical Geopotential
- -Arbitrary Equations of State

Linear Modes
- -No Spurious Stationary Modes
- -Good Dispersion Relationship
- -No Spurious Branches of Waves
- -No Inertial Modes

Accuracy
- -Taylor Series Sense
- -Convergence to Reference Solutions

Balanced Dynamics
- -No Spurious Vorticity Generation
- -Hydrostatic Balance
- -Steady Geostrophic Modes

Conservation
- -Mass
- -Energy
- -Entropy/Potential Temperature
- -Moisture/Tracers

Compatible Advection
- -Thermodynamic Variables
- -Tracers/Moisture

Efficiency
- -Strong/Weak Scalability
- -Time to Solution

Stability
- -No Hollingsworth Instability
- -Nonlinear Stability

Generality
- -Reversible Dynamics
- -Irreversible Dynamics

Other
- -Geometric Flexibility
- -Inactive Regions

Any mimetic spatial/temporal discretizations give these properties

These are a function of the specific choice of mimetic discretization and the implementation

1 Motivation and Overview

2 Reversible (Entropy-Conserving) Dynamics

3 Irreversible (Entropy-Generating) Dynamics

4 Summary and Outlook

Hamiltonian Formulation

Hamiltonian Formulation: Easily expresses conservation-especially total energy $\mathcal{H}$ and Casimirs $\mathcal{C}$ (total mass, total entropy, total buoyancy)

$$\frac{\partial \mathbf{x}}{\partial t} = \mathbb{J}\frac{\delta \mathcal{H}}{\delta \mathbf{x}} \qquad \mathbb{J} = -\mathbb{J}^T \qquad \mathbb{J}\frac{\delta \mathcal{C}}{\delta \mathbf{x}} = 0$$

$$\frac{d\mathcal{H}}{dt} = \left(\frac{\delta \mathcal{H}}{\delta \mathbf{x}}\right)^T \mathbb{J}\frac{\delta \mathcal{H}}{\delta \mathbf{x}} = -\left(\frac{\delta \mathcal{H}}{\delta \mathbf{x}}\right)^T \mathbb{J}\frac{\delta \mathcal{H}}{\delta \mathbf{x}} = 0$$

$$\frac{d\mathcal{C}}{dt} = \left(\frac{\delta \mathcal{C}}{\delta \mathbf{x}}\right)^T \mathbb{J}\frac{\delta \mathcal{H}}{\delta \mathbf{x}} = 0$$

This describes reversible (entropy-conserving) dynamics. I will discuss the extension to irreversible (entropy-generating) dynamics in the next section.

Spatial: Tensor Product Compatible Galerkin

$$\begin{tikzcd}
\mathbb{W}_0 \arrow[r, "d", "\nabla"'] & \mathbb{W}_1 \arrow[r, "d", "\nabla\times"'] & \mathbb{W}_2 \arrow[r, "d", "\nabla\cdot"'] & \mathbb{W}_3 \arrow[lll, bend left, dashed, "\nabla\cdot", "\delta"'] \arrow[ll, bend left, dashed, "\nabla\times", "\delta"'] \arrow[l, bend left, dashed, "\nabla", "\delta"']
\end{tikzcd}$$

$$(da^k, b^{k+1}) = (a^k, \delta b^{k+1})$$

Tensor Product Construction

Start: $\mathcal{A} \subset H^1 \xrightarrow{\frac{d}{dx}} \mathcal{B} \subset L_2$

$\mathbb{W}_0 = \mathcal{A} \otimes \mathcal{A} \otimes \mathcal{A} \subset H_1$

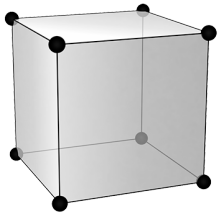
$\mathbb{W}_1 = (\mathcal{B} \otimes \mathcal{A} \otimes \mathcal{A})\,\hat{\mathbf{i}} + \cdots \subset H(curl)$

$\mathbb{W}_2 = (\mathcal{A} \otimes \mathcal{B} \otimes \mathcal{B})\,\hat{\mathbf{i}} + \cdots \subset H(div)$

$\mathbb{W}_3 = \mathcal{B} \otimes \mathcal{B} \otimes \mathcal{B} \subset L_2$

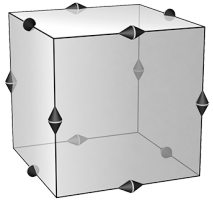
$\mathbb{CP} = \mathcal{B} \otimes \mathcal{B} \otimes \mathcal{A} = \mathbb{W}_2^v$

Exact sequence: $dd = 0$ **Hodge decomposition**: $\omega = d\alpha + \delta\beta + \gamma$



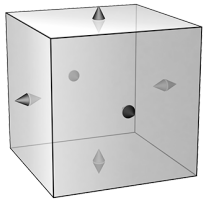
$\mathbb{W}_0 \subset H^1$

s



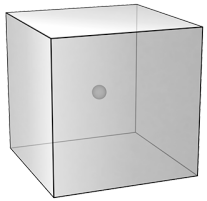
$\mathbb{W}_1 \subset H(curl)$

ζ, q



$\mathbb{W}_2 \subset H(div)$

$\mathbf{u}, \mathbf{v}$



$\mathbb{W}_3 \subset L_2$

ρ, S, s

Examples: mimetic spectral elements, isogeometric differential forms, compatible finite elements, **mimetic Galerkin differences (MGD_n)**

Temporal: Energy-Conserving Poisson Integrator

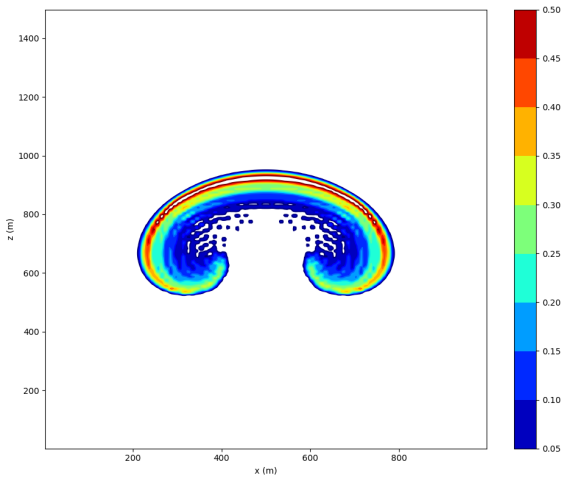
A **2nd-order**, fully **implicit**, **energy conserving** time integrator for Poisson systems of ODEs is:

$$
\begin{aligned}
\frac{\mathbf{x}^{n+1} - \mathbf{x}^{n}}{\Delta t} &= \widetilde{\mathbf{J}}\widetilde{\nabla\mathcal{H}} \\
\widetilde{\mathbf{J}} &= \mathbf{J}\left(\frac{\mathbf{x}^{n+1} + \mathbf{x}^{n}}{2}\right) \\
\widetilde{\nabla\mathcal{H}} &= \int \frac{\delta\mathcal{H}}{\delta\mathbf{x}}(\mathbf{x}^{n} + \tau(\mathbf{x}^{n+1} - \mathbf{x}^{n}))d\tau
\end{aligned}
$$

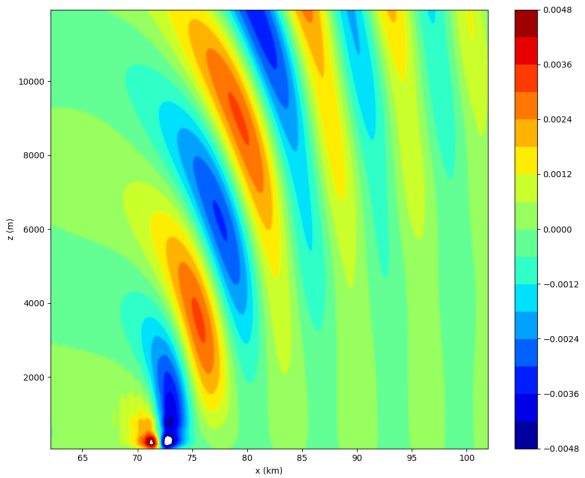
Evaluate the **discrete gradient** $\widetilde{\nabla\mathcal{H}}$ via a **quadrature rule**. Conserves **quadratic Casimirs** $\mathcal{C}$ and **arbitrary** $\mathcal{H}$. Details are in Cohen and Hairer (2011)

- Can **simplify Jacobian** to get a **semi-implicit** system without compromising energy conserving nature
- No CFL restriction due to sound waves or other fast motions

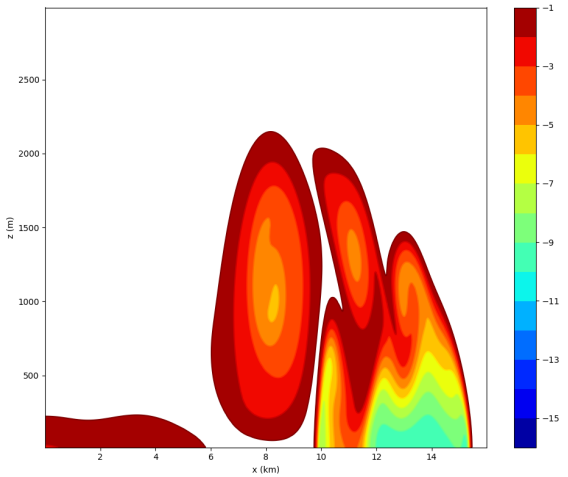
Compressible Euler Equations: Results



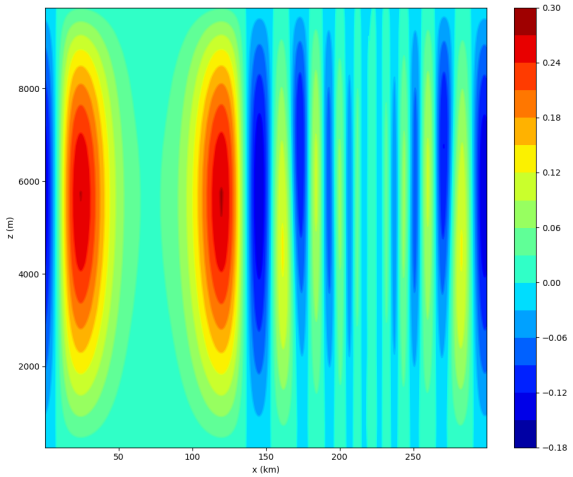
Rising Bubble



NH Mountain Wave



Density Current

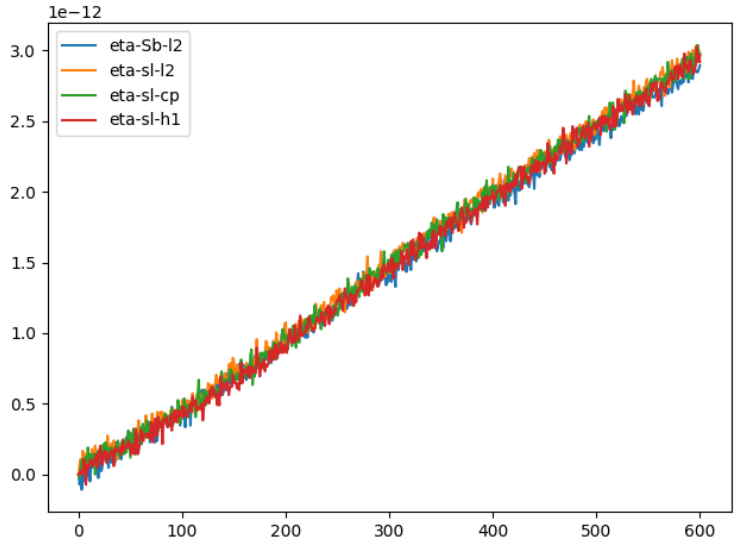


NH Gravity Wave

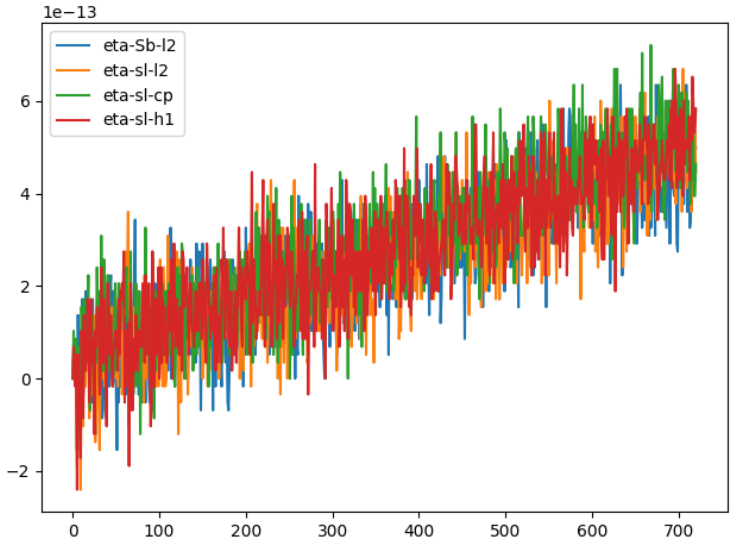
MGD-3, predict $S \in \mathbb{W}_3$, xz slice, 2nd order Poisson integrator (4pt quadrature), **no dissipation/subgrid model**, **centered flux** for surface integrals, simplified (semi-implicit) Jacobian

Can also predict $s \in \mathbb{W}_0/\mathbb{W}_3/\mathbb{CP}$ or θ or $\Theta = \rho\theta$, similar results

Compressible Euler Equations: Conservation



$(\mathcal{H} - \mathcal{H}_0)/\mathcal{H}_0 * 100.$
NH Gravity Wave



$(\mathcal{H} - \mathcal{H}_0)/\mathcal{H}_0 * 100.$
Rising Bubble

All variants are conserving total energy $\mathcal{H}$ to machine precision for both test cases (also $\mathcal{M}$ and $\mathcal{B}$, not shown)

1 Motivation and Overview

2 Reversible (Entropy-Conserving) Dynamics

3 Irreversible (Entropy-Generating) Dynamics

4 Summary and Outlook

Continuous Irreversible Dynamics

Consider a simple representation of **irreversible** subgrid turbulence:

$$\begin{aligned} \frac{\partial \mathbf{v}}{\partial t} + \cdots - \frac{1}{\rho}\nabla \cdot \sigma_{fr} &= 0 \\ \frac{\partial S}{\partial t} + \cdots + \frac{1}{T}\nabla \cdot \mathbf{j}_h - \frac{1}{T}\nabla \mathbf{u} : \sigma_{fr} &= 0 \end{aligned}$$

Key question: How to treat stress tensor σ_{fr} and heat flux $\mathbf{j}_h$?

Parameterization of σ_{fr} and $\mathbf{j}_h$

strains: E, I, J ; shears: F, G, H, gives trace-free and symmetric σ_{fr}

$$\sigma_{fr} = \begin{pmatrix} \kappa_m^h E + \kappa_m^v I & \kappa_m^h F & \kappa_m^v G \\ \kappa_m^h F & -\kappa_m^h E + \kappa_m^v J & \kappa_m^v H \\ \kappa_m^v G & \kappa_m^v H & -\kappa_m^h I - \kappa_m^v J \end{pmatrix}$$

$$\mathbf{j}_h = \begin{pmatrix} \kappa_s^h & 0 & 0 \\ 0 & \kappa_s^h & 0 \\ 0 & 0 & \kappa_s^v \end{pmatrix} \nabla T$$

Discrete Irreversible Dynamics

Spatial discretization (not shown) gives metriplectic system of ODEs

$$\frac{\partial \mathbf{x}}{\partial t} = \mathbf{M}(\mathbf{x}, \nabla\mathcal{H})\nabla\mathcal{S}$$

with $\mathbf{M}$ symmetric positive definite (**entropy generation**) and $\nabla\mathcal{H}^T\mathbf{M}(\mathbf{x}, \nabla\mathcal{H}) = 0$ (**energy conservation**)

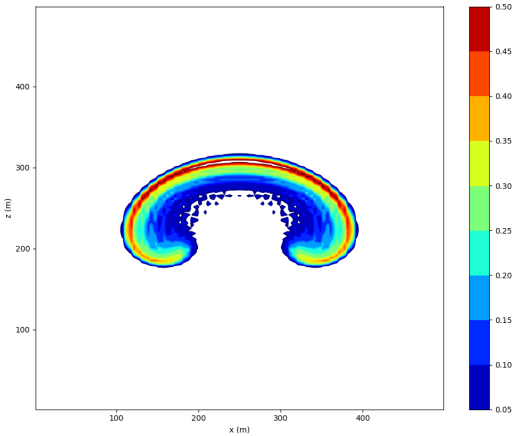
Temporal Discretization (Discrete Gradient)

Key idea: Evaluate $\mathbf{x}$ and $\nabla\mathcal{H}$ in $\mathbf{M}$ using same discrete gradient as for $\nabla\mathcal{H}$ and $\nabla\mathcal{S}$

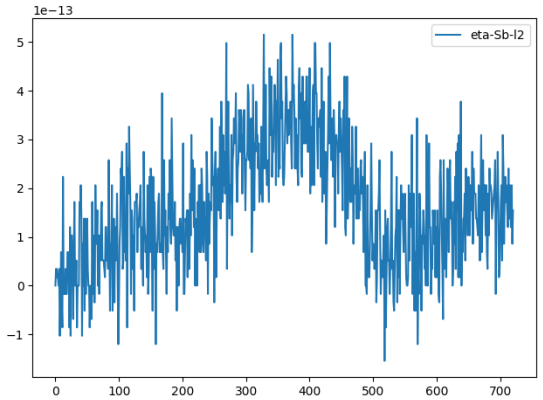
$$\frac{\partial \mathbf{x}}{\partial t} = \tilde{\mathbf{M}}(\tilde{\mathbf{x}}, \widetilde{\nabla\mathcal{H}})\widetilde{\nabla\mathcal{S}}$$

***There are more sophisticated ways to treat subgrid turbulence, but this is a reasonable first step that conserves energy and generates entropy**

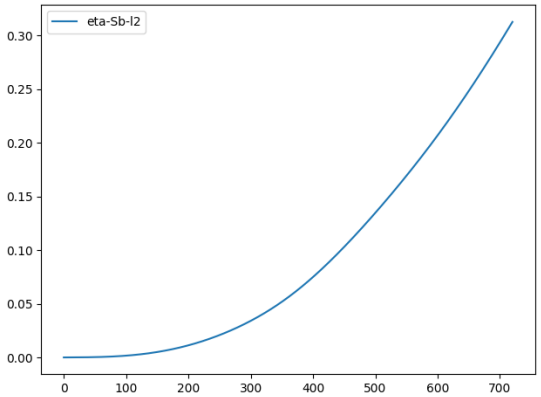
Rising Bubble Results



θ' at $T = 600$s



$(\mathcal{H} - \mathcal{H}_0)/\mathcal{H}_0 * 100.$



$(\mathcal{S} - \mathcal{S}_0)/\mathcal{S}_0 * 100.$

Exact (to machine-precision) conservation of total energy and generation of entropy with physics parameterizations and time discretization

100 x 200 mesh (1km x 2km domain, $\Delta x = \Delta z = 10$m), $\Delta t = 5$s
MGD-3, xz slice, 4pt quadrature for discrete gradients, **centered flux** for surface integrals, simplified (semi-implicit) Jacobian

1 Motivation and Overview

2 Reversible (Entropy-Conserving) Dynamics

3 Irreversible (Entropy-Generating) Dynamics

4 Summary and Outlook

Structure-Preserving Models of Geophysical Fluids

$$\begin{tikzcd} \mathbb{W}_0 \arrow[r, "d", "\nabla"'] & \mathbb{W}_1 \arrow[r, "d", "\nabla\times"'] \arrow[l, bend left, dashed, "\nabla\cdot", "\delta"'] & \mathbb{W}_2 \arrow[r, "d", "\nabla\cdot"'] \arrow[l, bend left, dashed, "\nabla\times", "\delta"'] & \mathbb{W}_3 \arrow[l, bend left, dashed, "\nabla", "\delta"'] \end{tikzcd}$$

$$(da^k, b^{k+1}) = (a^k, \delta b^{k+1})$$

Discrete deRham Complex

$$\frac{\mathbf{x}^{n+1} - \mathbf{x}^n}{\Delta t} = \widetilde{\mathbf{J}}\widetilde{\nabla\mathcal{H}} + \widetilde{\mathbf{M}}\widetilde{\nabla\mathcal{S}}$$

$$\mathcal{H}^{n+1} - \mathcal{H}^n = 0$$

$$\mathcal{S}^{n+1} - \mathcal{S}^n \geqslant 0$$

Quasi-Metriplectic Formulation

$\mathbb{W}_0 \subset H^1$ $\mathbb{W}_1 \subset H(curl)$ $\mathbb{W}_2 \subset H(div)$ $\mathbb{W}_3 \subset L_2$

This approach is quite general, and applies much more widely than just compressible Euler equations, or even geophysical fluids

Summary and Outlook

Summary

1. A **general framework** for structure-preserving discretizations exists: discretize a **bracket formulation** using **mimetic spatial discretization** and **energy-conserving metriplectic integrator**
2. For **atmospheric** models, one possible choice is **tensor-product Galerkin methods (MGD_n)** on **structured grids** and an **implicit** discrete gradient integrator
3. Choice of discretizations is highly **application-specific**

Outlook

1. **Turbulence** + **Multicomponent**/**Moisture**: Gassmann 2015/2018, SALT/LU? convected fluid microstructure? Multifluid? EDMF?
2. Improved **advection**: **Upwinding** (see Golo Wimmer Talk), monotonic?, semi-Lagrangian?
3. **Efficiency**: better **preconditioners** (see Thomas Gibson talk)

(Very Incomplete) List of References

1. C. Eldred and T. Dubos **Compatible Galerkin Discretization of the Compressible Euler Equations using Eulerian Coordinates**, in preparation
2. C. Eldred and F. Gay-Balmaz **Single and double generator bracket formulations of multicomponent fully compressible geophysical fluids with irreversible processes**, in preparation
3. C. Eldred, et. al. **A Quasi-Hamiltonian Discretization of the Thermal Shallow Water Equations**, *J. Comp. Physics*, 2018
4. C. Eldred and D. L. Le Roux. **Dispersion analysis of compatible Galerkin schemes for the 1D shallow water model** *J. Comp. Physics*, 2018
5. C. Eldred and D. L. Le Roux. **Dispersion analysis of compatible Galerkin schemes on quadrilaterals for shallow water models**, *J. Comp. Physics*, 2019
6. Cohen, D. and Hairer, E. **Linear energy-preserving integrators for Poisson systems**, *Bit Numer Math*, 2011
7. A. Natale, et. al. **Compatible finite element spaces for geophysical fluid dynamics**, *Dynamics and Statistics of the Climate System*, 2016
8. R.R. Hiemstra, D. Toshniwal, R.H.M. Huijsmans, M.I. Gerritsma. **High order geometric methods with exact conservation properties**, *J. Comp. Physics*, 2014
9. T. Melvin, et. al. **Choice of function spaces for thermodynamic variables in mixed finite element methods**, *QJRMS*, 2018
10. T. Melvin. **Dispersion analysis of the $P_n^C P_{n-1}^{DG}$ mixed finite element pair for atmospheric modelling**, *J. Comp. Physics*, 2018
11. P. Bochev, J. Hyman. **Principles of Mimetic Discretizations of Differential Operators**, *Compatible Spatial Discretizations*, 2006
12. A. Gassmann, H.-J. Herzog. **How is local material entropy production represented in a numerical model?**. *QJRMS*, 2015.
13. A. Gassmann. **Entropy production due to subgridscale thermal fluxes with application to breaking gravity waves**. *QJRMS*, 2018

Thanks for Listening! Questions?

Additional Slides

Irreversible Dynamics: Multicomponent, Multiphase

Irreversible processes of **momentum dissipation, diffusion, phase changes, thermal dissipation**:

$$\partial_t \mathbf{v} + \cdots - \frac{1}{\rho}\nabla \cdot \boldsymbol{\sigma}^{\mathrm{fr}} = 0$$

$$\partial_t \rho_i + \cdots + \nabla \cdot \mathbf{j}_{\mathrm{i}} - j_i = 0$$

$$\partial_t S + \cdots + \nabla \cdot \mathbf{j}_{\mathrm{s}} - \frac{1}{T}\boldsymbol{\sigma}^{\mathrm{fr}} : \nabla \mathbf{u} + \frac{1}{T}\mathbf{j}_{\mathrm{s}} \cdot \nabla T + \frac{1}{T}\sum_i (\mathbf{j}_{\mathrm{i}} \cdot \nabla \mu_i + j_i \mu_i) = 0$$

Conserve total energy $\mathcal{H}$ and **generate** entropy $\mathcal{S}$

$$\mathcal{H} = \int \rho \left[\frac{\mathbf{u} \cdot \mathbf{u}}{2} + \Phi + U(q_i, \alpha, s) \right] dx \qquad \mathcal{S} = \int S dx = \int \rho s dx$$

with appropriate choices for parameterizations of **thermodynamic fluxes** $\boldsymbol{\sigma}^{\mathrm{fr}}$, $\mathbf{j}_{\mathrm{i}}$, j_i, $\mathbf{j}_{\mathrm{s}}$in terms of **thermodynamic forces**
Def $\mathbf{u} = \frac{1}{2}(\nabla \mathbf{u} + \nabla^T \mathbf{u})$, ∇T, $\nabla \mu_i$, μ_i

Motivating science question

For barotropic vorticity equations*, possible to have numerical schemes with **good short-term trajectories** and **wrong (subtly) long-term statistics**; correct statistics requires **fully conservative (spatial and temporal)** schemes (ie. structure-preservation, see also well-known results from classical/Hamiltonian mechanics)

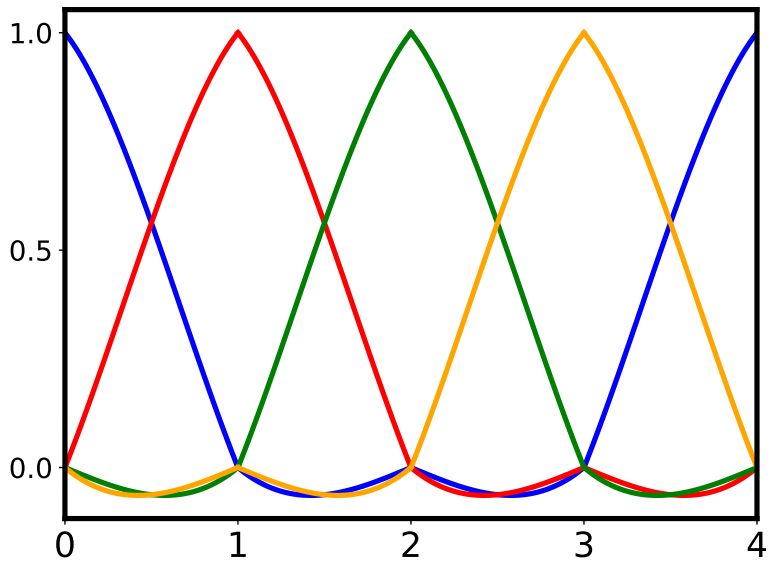
To what extend is this true for more complicated equations of geophysical fluid dynamics, especially forced-dissipative climate system?

To study this, need to know/develop:

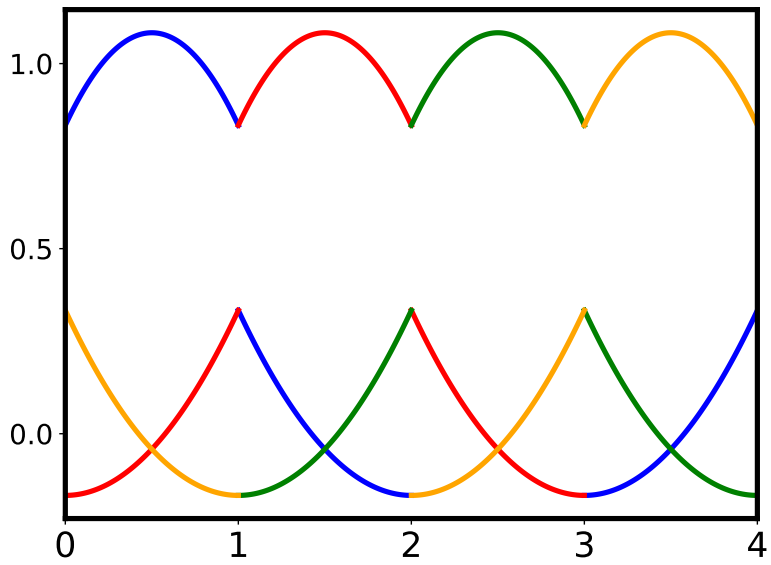
1. **Geometric structure** underlying forced-dissipative systems: **Metriplectic structure**
2. Numerical model that respects this structure: **mimetic spatial** and **metriplectic** temporal discretizations

* S. Dubinkina and J. Frank, Statistical Mechanics of Arakawa's Discretizations, JCP 2007

Mimetic Galerkin Differences (MGD_n)



$\mathcal{A} = GD_3 \subset H_1$ Space (1D)



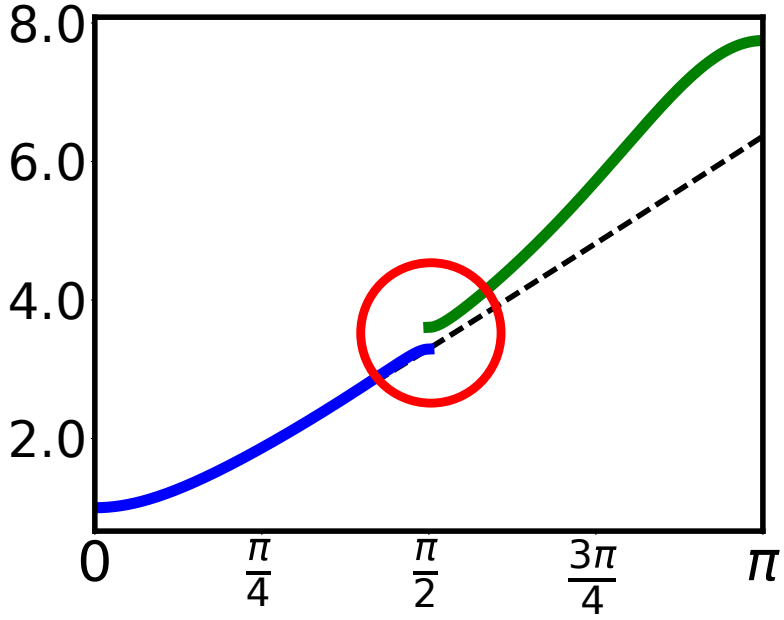
$\mathcal{B} = DGD_2 \subset L_2$ Space (1D)

- Higher-order by **increasing support** of basis functions
- **Single degree of freedom** per geometric entity → dofs are **identical** to finite-difference (physics and tracer transport coupling)
- Larger stencils (less local, efficiency concerns)

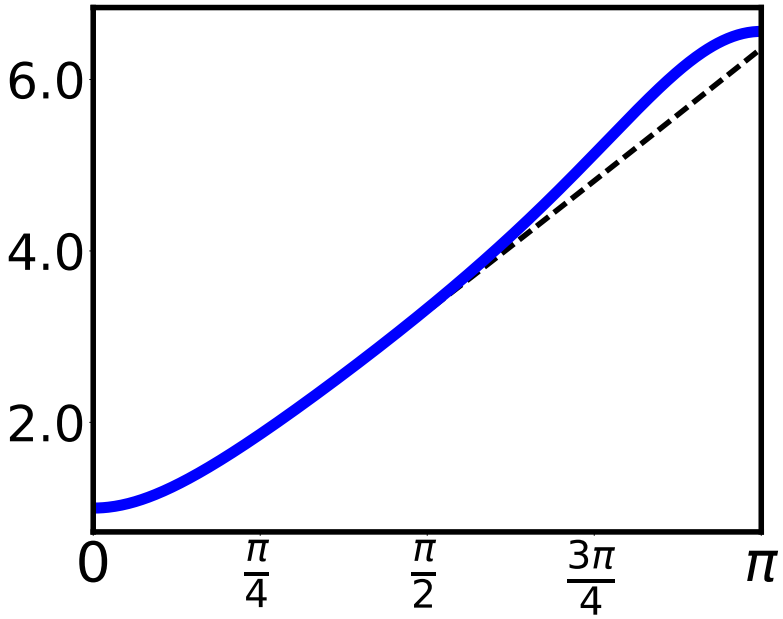
Combination of ideas from Banks and Hagstrom (2016) and Hiemstra et. al (2014); $n = 3$ spaces originally developed by Dubos and Kritsikis

$P_n^C - P_{n-1}^{DG}$ and MGD_n Dispersion Relationships

Inertia-Gravity Wave Dispersion Relationship (RSW, 1D)



$P_2^C - P_1^{DG}$



MGD_3

- $P_n^C - P_{n-1}^{DG}$: spectral gaps, maximal frequency overshoots (CFL condition)
- Can fix gaps with mass lumping, but equation dependent and doesn't work for 3rd order and higher
- MGD_n: Spectral gap is gone, overshoot reduced (longer explicit time steps)

More details on MGD_n and $P_n^C - P_{n-1}^{DG}$ dispersion relations in Eldred and Le Roux (2018), Melvin (2018)

Mimetic Spatial Discretizations

Primal Approach

- Constructs a **single** discrete deRham complex
- Represent Hodge star $\star$ and codifferential δ implicitly via integration by parts
- ex. compatible Galerkin methods (including FEEC)

$$\begin{tikzcd}
\mathbb{W}_0 \arrow[r, "d", "\nabla"'] & \mathbb{W}_1 \arrow[r, "d", "\nabla\times"'] & \mathbb{W}_2 \arrow[r, "d", "\nabla\cdot"'] & \mathbb{W}_3 \arrow[lll, bend left, dashed, "\nabla\cdot", "\delta"'] \arrow[ll, bend left, dashed, "\nabla\times", "\delta"'] \arrow[l, bend left, dashed, "\nabla", "\delta"']
\end{tikzcd}$$

$$(da^k, b^{k+1}) = (a^k, \delta b^{k+1})$$

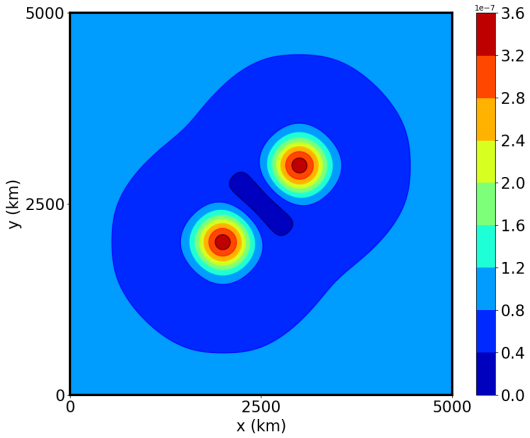
Primal-Dual Approach

- Constructs a **pair** of discrete deRham complexes
- Represent $\star$ and δ explicitly
- ex. discrete exterior calculus, primal-dual mixed finite elements

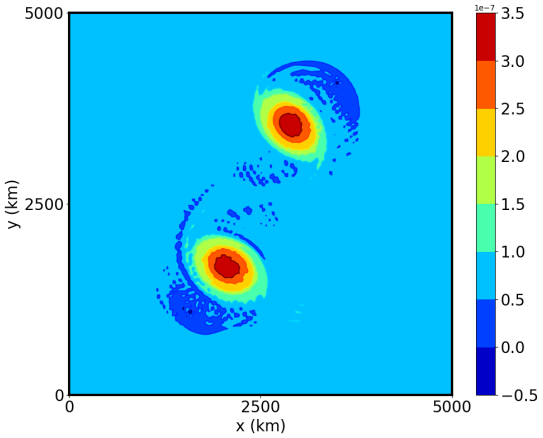
$$\begin{tikzcd}
\mathbb{W}_0 \arrow[r, "d", "\vec{\nabla}"'] \arrow[d, "*"] & \mathbb{W}_1 \arrow[r, "d", "\vec{\nabla}\times"'] \arrow[d, "*"] & \mathbb{W}_2 \arrow[r, "d", "\vec{\nabla}\cdot"'] \arrow[d, "*"] & \mathbb{W}_3 \arrow[d, "*"] \\
\mathbb{W}^3 & \mathbb{W}^2 \arrow[l, "d", "\vec{\nabla}\cdot"'] & \mathbb{W}^1 \arrow[l, "d", "\vec{\nabla}\times"'] & \mathbb{W}^0 \arrow[l, "d", "\vec{\nabla}"']
\end{tikzcd}$$

Double Vortex

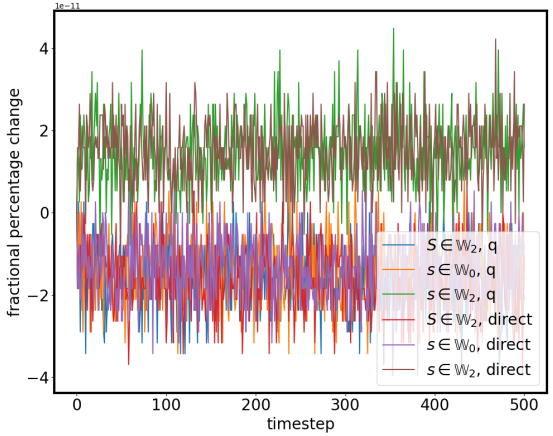
MGD-3 (5pt quadrature), 2nd order Poisson integrator (2pt quadrature), **no dissipation/subgrid model**, **centered flux** for surface integrals, **simplified Jacobian**, showing $s \in \mathbb{W}_3$ with direct PV flux term variant



$N = 0$



$N = 250$



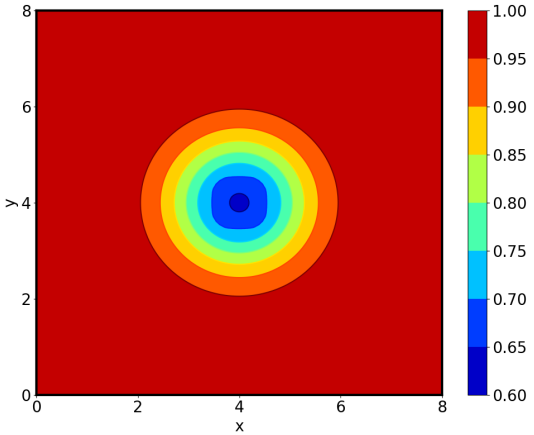
$(\mathcal{H} - \mathcal{H}_0)/\mathcal{H}_0 * 100.$

direct cascade, small-scale features

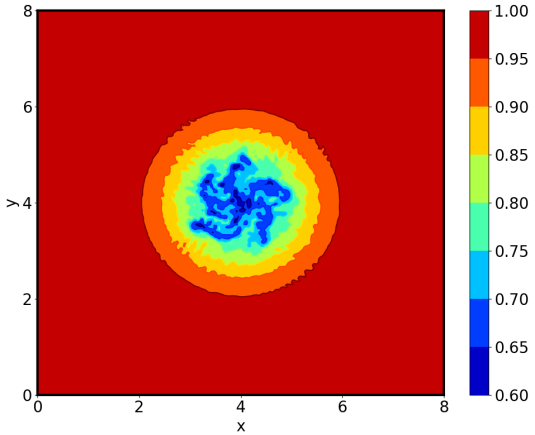
robust, conservation to machine precision

Thermal Instability

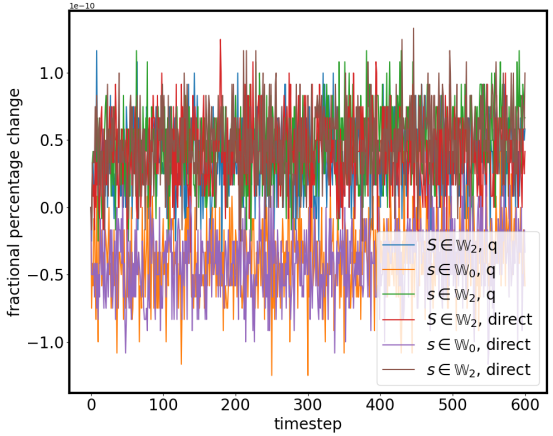
MGD-3 (5pt quadrature), 2nd order Poisson integrator (2pt quadrature), **no dissipation/subgrid model**, **centered flux** for surface integrals, **simplified Jacobian**, showing $s \in \mathbb{W}_3$ with direct PV flux term variant



$N = 0$



$N = 400$



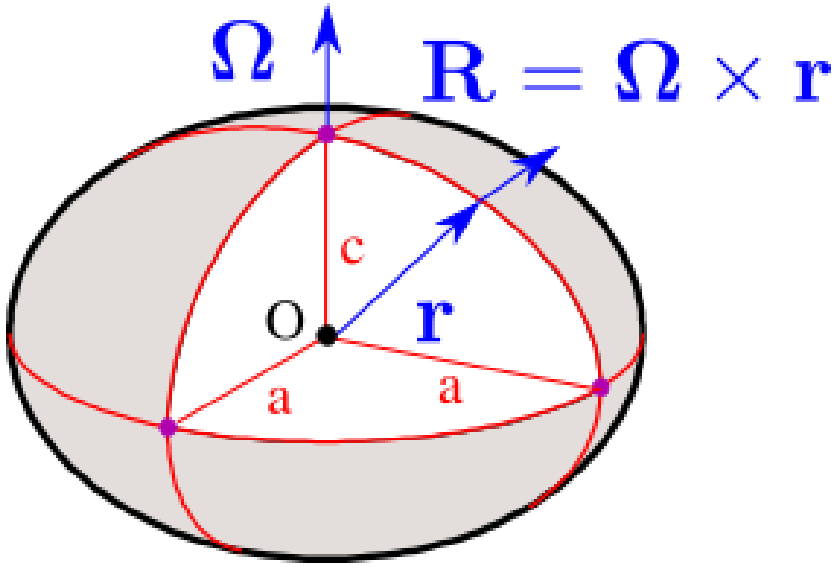
$(\mathcal{H} - \mathcal{H}_0)/\mathcal{H}_0 * 100.$

complicated nonlinear flow, saturation of instability

robust, conservation to machine precision

Domain and Variables

Eventual Target: Fully Compressible Euler in Elliptic Domain = Deep, Nonhydrostatic, Elliptical Atmospheres



- **Material surfaces** ($\mathbf{u} \cdot \hat{\mathbf{n}} = 0$) at domain boundaries
- Variables are **density** ρ, the **absolute velocity** $\mathbf{v} = \mathbf{u} + \mathbf{R}$ and either the **entropy*** s or the **mass-weighted** entropy* $S = \rho s$
- Relative velocity $\mathbf{u}$, rotational velocity $\mathbf{R}$ and rotation vector $\mathbf{\Omega}$

*Can use potential temperature θ instead of s and mass-weighted potential temperature $\Theta = \rho\theta$ instead of S (advantages for ideal gas)

Currently software framework only supports single block grid

Hamiltonian and Functional Derivatives

$$\mathcal{H}[\rho, \mathbf{v}, S] = \langle \rho, K \rangle + \langle \rho, U \rangle + \langle \rho, \Phi \rangle$$

$$\begin{aligned}
\left\langle \hat{\rho}, \frac{\delta \mathcal{H}}{\delta \rho} \right\rangle &:= \langle \hat{\rho}, B \rangle = \langle \hat{\rho}, K + \Phi + U + p\alpha - sT \rangle \\
\left\langle \hat{\mathbf{v}}, \frac{\delta \mathcal{H}}{\delta \mathbf{v}} \right\rangle &:= \langle \hat{\mathbf{v}}, \mathbf{F} \rangle = \langle \hat{\mathbf{v}}, \rho\, \mathbf{u} \rangle \\
\left\langle \hat{S}, \frac{\delta \mathcal{H}}{\delta S} \right\rangle &:= \left\langle \hat{S}, T \right\rangle
\end{aligned}$$

where $K = \frac{1}{2}(\mathbf{v} - \mathbf{R}) \cdot (\mathbf{v} - \mathbf{R})$, $\alpha = \frac{1}{\rho}$, $T = \frac{\partial U}{\partial s}$, $p = -\frac{\partial U}{\partial \alpha}$

- $\langle , \rangle$ is the L_2 inner product
- Internal energy $U = U(\alpha, s)$ from **arbitrary** equation of state
- **Different choices** of $\mathbf{R}$, geopotential Φ and underlying spatial metric give shallow atmosphere, traditional and spherical **approximations**

Discrete Equations of Motion

$$\left\langle \hat{\rho}, \frac{\partial \rho}{\partial t} \right\rangle + \langle \hat{\rho}, \nabla \cdot \mathbf{F} \rangle = 0$$

$$\left\langle \hat{\mathbf{v}}, \frac{\partial \mathbf{v}}{\partial t} \right\rangle + \left\langle \nabla_H \times \left(\frac{\mathbf{F}}{\rho} \times \hat{\mathbf{v}} \right), \mathbf{v} \right\rangle + \left\langle \left[\left(\frac{\mathbf{F}}{\rho} \times \hat{\mathbf{v}} \right) \times \hat{\mathbf{n}} \right], \{\mathbf{v}\} + c_f [\mathbf{v}] \right\rangle_{\Gamma_I}$$

$$+ \left\langle \left(\frac{\mathbf{F}}{\rho} \times \hat{\mathbf{v}} \right) \times \hat{\mathbf{n}}, \mathbf{v} \right\rangle_{\Gamma_E} - \langle \nabla \cdot \hat{\mathbf{v}}, B \rangle + \langle s\, \hat{\mathbf{v}}, \nabla_H T \rangle - \langle [T\, \hat{\mathbf{v}}, \hat{\mathbf{n}}], \{s\} + c_f [s] \rangle_{\Gamma_I} = 0$$

$$\left\langle \hat{S}, \frac{\partial S}{\partial t} \right\rangle - \left\langle \nabla_H \hat{S}, s\, \mathbf{F} \right\rangle + \left\langle [\hat{S}\, \mathbf{F}, \hat{\mathbf{n}}], \{s\} + c_f [s] \right\rangle_{\Gamma_I} = 0$$

- $\mathbf{u} \cdot \hat{\mathbf{n}} = \mathbf{F} \cdot \hat{\mathbf{n}} = 0$ on boundary
- **Diagnose** s, $\mathbf{F}$, T
- **Substitute** B

- The ρ equation holds **pointwise**
- 6 equations in 6 unknowns: $(\rho, \mathbf{v}, S, s, \mathbf{F}, T)$

Diagnose s with $\langle \hat{s}, \rho s \rangle = \langle \hat{s}, S \rangle$

$[x] = x^+ - x^-$ facet jump
$[\mathbf{x}, \hat{\mathbf{n}}] = \mathbf{x}^+ \hat{\mathbf{n}}^+ + \mathbf{x}^- \hat{\mathbf{n}}^-$ scalar facet jump
$\{x\} = \frac{x^+ + x^-}{2}$ facet average
$\langle \rangle_{\Gamma_I}$ interior facet integral
$\langle \rangle_{\Gamma_E}$ exterior facet integral
∇_H local to an element

stabilization term c_f

$$\begin{cases} \frac{\alpha}{2} & \text{if } \mathbf{F} \cdot \hat{\mathbf{n}} > 0 \\ -\frac{\alpha}{2} & \text{if } \mathbf{F} \cdot \hat{\mathbf{n}} < 0 \end{cases}$$

$\alpha = 0 \rightarrow$ centered
$\alpha = 1 \rightarrow$ upwind

Conservation Properties

Variant	$\mathcal{M}$	$\mathcal{B}$	$\mathcal{H}$
A: $S \in \mathbb{W}_3$	$\langle \rho, 1 \rangle$	$\langle 1, S \rangle$	$\frac{1}{2}\langle \rho\,\mathbf{u}, \mathbf{u} \rangle + \left\langle \rho, U(\frac{1}{\rho}, \frac{S}{\rho}) \right\rangle + \langle \rho, \Phi \rangle$
B1: $s \in \mathbb{W}_0$	$\langle \rho, 1 \rangle$	$\langle \rho', s \rangle$	$\frac{1}{2}\langle \rho\,\mathbf{u}, \mathbf{u} \rangle + \left\langle \rho, U(\frac{1}{\rho}, s) \right\rangle + \langle \rho, \Phi \rangle$
B2: $s \in \mathbb{CP}$	$\langle \rho, 1 \rangle$	$\langle \rho', s \rangle$	$\frac{1}{2}\langle \rho\,\mathbf{u}, \mathbf{u} \rangle + \left\langle \rho, U(\frac{1}{\rho}, s) \right\rangle + \langle \rho, \Phi \rangle$
B3: $s \in \mathbb{W}_3$	$\langle \rho, 1 \rangle$	$\langle \rho, s \rangle$	$\frac{1}{2}\langle \rho\,\mathbf{u}, \mathbf{u} \rangle + \left\langle \rho, U(\frac{1}{\rho}, s) \right\rangle + \langle \rho, \Phi \rangle$

$\langle \hat{s}, \rho' \rangle = \langle \hat{s}, \rho \rangle$ with ρ' in the same space as s

Form of **Hamiltonian (total energy)** $\mathcal{H}$ and **Casimirs** $\mathcal{C}$ (mass $\mathcal{M}$ and mass-weighted entropy $\mathcal{B}$) conserved by the different variants

Casimirs $\mathcal{C}$: $\{\mathcal{C}, \mathcal{A}\} = 0 \quad \forall \mathcal{A}$

Hamiltonian $\mathcal{H}$: $\{\mathcal{A}, \mathcal{B}\} = -\{\mathcal{B}, \mathcal{A}\} \rightarrow \{\mathcal{H}, \mathcal{H}\} = -\{\mathcal{H}, \mathcal{H}\} = 0$

Other References

1. H. Heumann, et. al. **Stabilized Galerkin for transient advection of differential forms**, *Discrete & Continuous Dynamical Systems*, 2015
2. A. McRae, C. Cotter. **Energy- and enstrophy-conserving schemes for the shallow-water equations, based on mimetic finite elements**, *QJRMS*, 2014
3. J.W. Banks, T. Hagstrom. **On Galerkin difference methods**, *J. Comp. Physics*, 2016
4. J. Shipton et. al. **Higher-order compatible finite element schemes for the nonlinear rotating shallow water equations on the sphere**. arxiv
5. C. Cotter, J. Shipton. **Mixed finite elements for numerical weather prediction**, *J. Comp. Physics*, 2012
6. H.Yamazaki, et. al. **Vertical slice modelling of nonlinear Eady waves using a compatible finite element method**, *J. Comp. Physics*, 2017
7. A. Natale, C. Cotter. **A variational $H(div)$ finite-element discretization approach for perfect incompressible fluids**, *IMA Journal of Numerical Analysis*, 2017
8. C. Cotter, J. Thuburn. **A finite element exterior calculus framework for the rotating shallow-water equations**, *J. Comp. Physics*, 2014

Themis Software Framework

Themis Software Stack

(Non)linear variational problems in UFL plus problem solving lanuage (similar to FEniCS/Firedrake)

Form, Arguments, Coefficients, FiniteElement

Mesh, FunctionSpace, Field, EssentialBC

TSFC

Loop Nests

Themis (PETSc/petsc4py)

COFFEE

Optimized Local Assembly Kernels

Mat, Vec, DMDA, DMComposite KSP, SNES

Global Assembly and Solution

Themis is a software framework built on top of PETSc and designed for **automated, high-performance, parallel** discretization of **variational forms** with **tensor-product Galerkin** methods on **block-structured** grids. Shares design philosophy and components (UFL/TSFC/COFFEE) with Firedrake/FEniCS.

What is Themis?

1. PETSc-based software framework (written in Python and C)
2. Parallel, high-performance, automated discretization of variational forms
3. Tensor-product Galerkin methods on block-structured grids
4. Uses UFL/COFFEE/TSFC from Firedrake project
5. Enables rapid prototyping and experimentation

Themis is online at `https://github.com/celdred/themis`
Firedrake is at `http://www.firedrakeproject.org/`

Design Principles

1. Leverage existing software packages: PETSc, petsc4py, Numpy, Sympy, UFL, COFFEE, TSFC, ...
2. Restrict to a subset of methods: tensor-product Galerkin methods on block-structured grids
3. Similar in spirit and high-level design to FEniCS/Firedrake (shares UFL/COFFEE/TSFC)
4. Access to symbolic representation of forms: automatic adjoints and derivatives, seamless switching between assembled and matrix-free, clever physics-based preconditioners, many other advantages
5. Intended to offer "good enough" performance for many science applications (prototyping atmospheric dynamical cores is initial target application)

Example Code: H^1 Helmholtz (in Firedrake, Themis and FEniCS very similar)

```
mesh = UnitSquareMesh(10, 10)
V = FunctionSpace(mesh, "CG", 1)

u = TrialFunction(V)
v = TestFunction(V)

x, y = SpatialCoordinate(mesh)
f = (1+8*pi*pi)*cos(x*pi*2)*cos(y*pi*2)

a = (dot(grad(v), grad(u)) + v * u) * dx
L = f * v * dx

u = Function(V)

solve(a == L, u)
```

Current and Future Capabilities

1. Support for multiblock* structured grids in 1, 2 and 3 dimensions
2. Parallelism through MPI
3. Arbitrary curvilinear mappings between physical and reference space, including support for manifolds*
4. Support for mimetic Galerkin difference elements, $Q_r^- \Lambda^k$ elements (both Lagrange and Bernstein basis) and mimetic spectral elements (single-grid version only): plus mixed, vector, tensor and standard function spaces on those elements
5. Essential and periodic boundary conditions
6. Facet and volume integrals
7. Matrix-free operator action instead of assembly
8. Linear and nonlinear variational problems
9. Python/UFL-based preconditioners*

*- *work in progress*