Structure-preserving models of geophysical fluids

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Outline of Talk

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

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

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

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

#### Stability
- No Hollingsworth Instability
- Nonlinear Stability

#### Generality
- Reversible Dynamics
- Irreversible Dynamics

#### Other
- Geometric Flexibility
- Inactive Regions

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

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

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

#### Compatible Advection
- Thermodynamic Variables
- Tracers/Moisture

---

**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:
   \[
   \frac{\partial \mathbf{x}}{\partial t} = \mathbf{J}(\mathbf{x}) \frac{\delta \mathcal{H}}{\delta \mathbf{x}}(\mathbf{x}) + \mathbf{M}(\mathbf{x}) \frac{\delta \mathcal{S}}{\delta \mathbf{x}}(\mathbf{x})
   \]

2. Discretize space with a mimetic discretization scheme →
   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

   \[
   \frac{\mathbf{x}^{n+1} - \mathbf{x}^n}{\Delta t} = \tilde{\mathbf{J}}(\mathbf{x}^{n+1}, \mathbf{x}^n) \tilde{\nabla} \mathcal{H}(\mathbf{x}^{n+1}, \mathbf{x}^n) + \tilde{\mathbf{M}}(\mathbf{x}^{n+1}, \mathbf{x}^n) \tilde{\nabla} \mathcal{S}(\mathbf{x}^{n+1}, \mathbf{x}^n)
   \]

This gives most of the properties → choose specific mimetic
spatial and temporal discretizations to get the rest
What properties do we get? What remains?

Realistic Simulations

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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: Easily expresses conservation—especially total energy $H$ and Casimirs $C$ (total mass, total entropy, total buoyancy)

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

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

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

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

Tensor Product Construction

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

\[
\begin{align*}
W_0 & \to W_1 \to W_2 \to W_3 \\
\nabla & \to \nabla \times \to \nabla \cdot \\
\nabla \cdot & \to \nabla \times \to \nabla \\
\delta & \to \delta \to \delta \\
(d\alpha^k, b^{k+1}) &= (a^k, \delta b^{k+1})
\end{align*}
\]

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

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

\[
\begin{align*}
W_0 & \subset H^1 \\
W_1 & \subset H(\text{curl}) \\
W_2 & \subset H(\text{div}) \\
W_3 & \subset L_2 \\
\end{align*}
\]

\( s, \zeta, q, u, v, \rho, S, s \)
A 2nd-order, fully implicit, energy conserving time integrator for Poisson systems of ODEs is:

\[
\frac{x^{n+1} - x^n}{\Delta t} = \tilde{J} \tilde{\nabla} H
\]

\[
\tilde{J} = J\left(\frac{x^{n+1} + x^n}{2}\right)
\]

\[
\tilde{\nabla} H = \int \frac{\delta H}{\delta x} (x^n + \tau(x^{n+1} - x^n)) d\tau
\]

Evaluate the discrete gradient \( \tilde{\nabla} H \) via a quadrature rule. Conserves quadratic Casimirs \( C \) and arbitrary \( H \). 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

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

Can also predict $s \in \mathcal{W}_0/\mathcal{W}_3/C\mathcal{P}$ or $\theta$ or $\Theta = \rho\theta$, similar results
Compressible Euler Equations: Conservation

\[ \frac{(\mathcal{H} - \mathcal{H}_0)}{\mathcal{H}_0} \times 100. \]
NH Gravity Wave

\[ \frac{(\mathcal{H} - \mathcal{H}_0)}{\mathcal{H}_0} \times 100. \]
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

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

\[
\frac{\partial \mathbf{v}}{\partial t} + \cdots - \frac{1}{\rho} \nabla \cdot \sigma_{fr} = 0
\]

\[
\frac{\partial S}{\partial t} + \cdots + \frac{1}{T} \nabla \cdot \mathbf{j}_h - \frac{1}{T} \nabla \mathbf{u} : \sigma_{fr} = 0
\]

**Key question**: How to treat stress tensor \( \sigma_{fr} \) and heat flux \( \mathbf{j}_h \)?

**Parameterization of \( \sigma_{fr} \) and \( \mathbf{j}_h \)**

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

\[
\sigma_{fr} = \begin{pmatrix}
\kappa^h_m E + \kappa^v_m I & \kappa^h_m F & \kappa^v_m G \\
\kappa^h_m F & -\kappa^h_m E + \kappa^v_m J & \kappa^v_m H \\
\kappa^v_m G & \kappa^v_m H & -\kappa^h_m I - \kappa^v_m J
\end{pmatrix}
\]

\[
\mathbf{j}_h = \begin{pmatrix}
\kappa^h_s & 0 & 0 \\
0 & \kappa^h_s & 0 \\
0 & 0 & \kappa^v_s
\end{pmatrix} \nabla T
\]
Spatial discretization (not shown) gives metriplectic system of ODEs

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

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 \( \nabla S \)

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

*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

\( \theta' \text{ at } T = 600s \) \hspace{1cm} \left( \mathcal{H} - \mathcal{H}_0 \right)/\mathcal{H}_0 \times 100. \hspace{1cm} \left( S - S_0 \right)/S_0 \times 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, \( \Delta x = \Delta z = 10m \)), \( \Delta t = 5s \)
MGD-3, xz slice, 4pt quadrature for discrete gradients, centered flux for surface integrals, simplified (semi-implicit) Jacobian
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Structure-Preserving Models of Geophysical Fluids

Discrete deRham Complex

\[
\begin{align*}
\nabla & \rightarrow \nabla \times & \nabla \cdot \\
W_0 & \rightarrow W_1 & W_2 & \rightarrow W_3
\end{align*}
\]

\[
\begin{align*}
\nabla \cdot & \rightarrow \nabla \times & \nabla & \\
\delta & \rightarrow \delta & \delta &
\end{align*}
\]

\[
(d a^k, b^{k+1}) = (a^k, \delta b^{k+1})
\]

Quasi-Metriplectic Formulation

\[
\frac{x^{n+1} - x^n}{\Delta t} = \tilde{J} \nabla \mathcal{H} + \tilde{M} \nabla S
\]

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

\[
S^{n+1} - S^n \geq 0
\]

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


2. Improved advection: Upwinding (see Golo Wimmer Talk), monotonic?, semi-Lagrangian?

3. Efficiency: better preconditioners (see Thomas Gibson talk)

C. Eldred and F. Gay-Balmaz. **Single and double generator bracket formulations of multicomponent fully compressible geophysical fluids with irreversible processes**, in preparation


C. Eldred and D. L. Le Roux. **Dispersion analysis of compatible Galerkin schemes for the 1D shallow water model** *J. Comp. Physics*, 2018

C. Eldred and D. L. Le Roux. **Dispersion analysis of compatible Galerkin schemes on quadrilaterals for shallow water models**, *J. Comp. Physics*, 2019

Cohen, D. and Hairer, E. **Linear energy-preserving integrators for Poisson systems**, *Bit Numer Math*, 2011

A. Natale, et. al. **Compatible finite element spaces for geophysical fluid dynamics**, *Dynamics and Statistics of the Climate System*, 2016


T. Melvin, et. al. **Choice of function spaces for thermodynamic variables in mixed finite element methods**, *QJRMS*, 2018

T. Melvin. **Dispersion analysis of the $P_n^C P_{n-1}^{DG}$ mixed finite element pair for atmospheric modelling**, *J. Comp. Physics*, 2018


A. Gassmann, H.-J. Herzog. **How is local material entropy production represented in a numerical model?** *QJRMS*, 2015.

A. Gassmann. **Entropy production due to subgridscale thermal fluxes with application to breaking gravity waves**. *QJRMS*, 2018

**Thanks for Listening! Questions?**
Additional Slides
Irreversible processes of momentum dissipation, diffusion, phase changes, thermal dissipation:

\[
\begin{align*}
\partial_t \mathbf{v} + \cdots - \frac{1}{\rho} \nabla \cdot \mathbf{\sigma}^\text{fr} &= 0 \\
\partial_t \rho_i + \cdots + \nabla \cdot \mathbf{j}_i - j_i &= 0 \\
\partial_t S + \cdots + \nabla \cdot \mathbf{j}_s - \frac{1}{T} \mathbf{\sigma}^\text{fr} : \nabla \mathbf{u} + \frac{1}{T} \mathbf{j}_s \cdot \nabla T + \frac{1}{T} \sum_i (\mathbf{j}_i \cdot \nabla \mu_i + j_i \mu_i) &= 0
\end{align*}
\]

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

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

with appropriate choices for parameterizations of thermodynamic fluxes $\mathbf{\sigma}^\text{fr}$, $\mathbf{j}_i$, $j_i$, $\mathbf{j}_s$ in terms of thermodynamic forces

$\text{Def } \mathbf{u} = \frac{1}{2} (\nabla \mathbf{u} + \nabla^T \mathbf{u}), \nabla T, \nabla \mu_i, \mu_i$
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 ($MGD_n$)

\[ \mathcal{A} = GD_3 \subset H_1 \text{ Space (1D)} \quad \mathcal{B} = DGD_2 \subset L_2 \text{ Space (1D)} \]

- 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)**

- \( P_2^C - P_1^{DG} \): 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 $\delta$ implicitly via integration by parts
- ex. compatible Galerkin methods (including FEEC)

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

$$
\begin{align*}
W_0 & \rightarrow W_1 \rightarrow W_2 \rightarrow W_3 \\
\nabla & \rightarrow \nabla \times \rightarrow \nabla \cdot \\
\delta & \rightarrow \delta \rightarrow \delta \\
(d\alpha^k, \beta^{k+1}) & = (\alpha^k, \delta \beta^{k+1})
\end{align*}
$$
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

\[ N = 0 \]
\[ N = 250 \]
\[ \frac{\mathcal{H} - \mathcal{H}_0}{\mathcal{H}_0} \times 100. \]

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

\[ N = 0 \quad \text{complicated nonlinear flow, saturation of instability} \]

\[ N = 400 \quad \text{robust, conservation to machine precision} \]
Eventual Target: Fully Compressible Euler in Elliptic Domain
= Deep, Nonhydrostatic, Elliptical Atmospheres

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

*Can use potential temperature \(\theta\) 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

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

\[ \langle \hat{\rho}, \frac{\delta \mathcal{H}}{\delta \rho} \rangle := \langle \hat{\rho}, B \rangle = \langle \hat{\rho}, K + \Phi + U + p\alpha - sT \rangle \]

\[ \langle \hat{\mathbf{v}}, \frac{\delta \mathcal{H}}{\delta \mathbf{v}} \rangle := \langle \hat{\mathbf{v}}, \mathbf{F} \rangle = \langle \hat{\mathbf{v}}, \rho \mathbf{u} \rangle \]

\[ \langle \hat{S}, \frac{\delta \mathcal{H}}{\delta S} \rangle := \langle \hat{S}, T \rangle \]

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

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

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

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

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

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

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

Diagnose \( s \) with \( \left\langle \hat{s}, \rho s \right\rangle = \left\langle \hat{s}, S \right\rangle \)

- Stabilization term \( c_f \)

\[
\begin{align*}
\alpha &= \frac{\alpha}{2} \quad \text{if } \mathbf{F} \cdot \hat{\mathbf{n}} > 0 \\
\alpha &= -\frac{\alpha}{2} \quad \text{if } \mathbf{F} \cdot \hat{\mathbf{n}} < 0 \\
\alpha &= 0 \rightarrow \text{centered} \\
\alpha &= 1 \rightarrow \text{upwind}
\end{align*}
\]

\[
[x] = x^+ - x^- \quad \text{facet jump} \\
[x, \hat{\mathbf{n}}] = x^+ \hat{\mathbf{n}}^+ + x^- \hat{\mathbf{n}}^- \quad \text{scalar facet jump} \\
\{x\} = \frac{x^++x^-}{2} \quad \text{facet average} \\
\left\langle \right\rangle_{\Gamma_I} \quad \text{interior facet integral} \\
\left\langle \right\rangle_{\Gamma_E} \quad \text{exterior facet integral} \\
\nabla_H \quad \text{local to an element}
\]
### Conservation Properties

<table>
<thead>
<tr>
<th>Variant</th>
<th>$\mathcal{M}$</th>
<th>$\mathcal{B}$</th>
<th>$\mathcal{H}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A: $S \in \mathbb{W}_3$</td>
<td>$\langle \rho, 1 \rangle$</td>
<td>$\langle 1, S \rangle$</td>
<td>$\frac{1}{2} \langle \rho \mathbf{u}, \mathbf{u} \rangle + \langle \rho, U(\frac{1}{\rho}, \frac{S}{\rho}) \rangle + \langle \rho, \Phi \rangle$</td>
</tr>
<tr>
<td>B1: $s \in \mathbb{W}_0$</td>
<td>$\langle \rho, 1 \rangle$</td>
<td>$\langle \rho', s \rangle$</td>
<td>$\frac{1}{2} \langle \rho \mathbf{u}, \mathbf{u} \rangle + \langle \rho, U(\frac{1}{\rho}, s) \rangle + \langle \rho, \Phi \rangle$</td>
</tr>
<tr>
<td>B2: $s \in \mathbb{CP}$</td>
<td>$\langle \rho, 1 \rangle$</td>
<td>$\langle \rho', s \rangle$</td>
<td>$\frac{1}{2} \langle \rho \mathbf{u}, \mathbf{u} \rangle + \langle \rho, U(\frac{1}{\rho}, s) \rangle + \langle \rho, \Phi \rangle$</td>
</tr>
<tr>
<td>B3: $s \in \mathbb{W}_3$</td>
<td>$\langle \rho, 1 \rangle$</td>
<td>$\langle \rho, s \rangle$</td>
<td>$\frac{1}{2} \langle \rho \mathbf{u}, \mathbf{u} \rangle + \langle \rho, U(\frac{1}{\rho}, s) \rangle + \langle \rho, \Phi \rangle$</td>
</tr>
</tbody>
</table>

$\langle \hat{s}, \rho' \rangle = \langle \hat{s}, \rho \rangle$ with $\rho'$ 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** $\mathcal{H}$: $\{\mathcal{A}, \mathcal{B}\} = -\{\mathcal{B}, \mathcal{A}\} \rightarrow \{\mathcal{H}, \mathcal{H}\} = -\{\mathcal{H}, \mathcal{H}\} = 0$


4. J. Shipton et. al. *Higher-order compatible finite element schemes for the nonlinear rotating shallow water equations on the sphere*. arxiv


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/
Leverage existing software packages: PETSc, petsc4py, Numpy, Sympy, UFL, COFFEE, TSFC, ...

Restrict to a subset of methods: tensor-product Galerkin methods on block-structured grids

Similar in spirit and high-level design to FEniCS/Firedrake (shares UFL/COFFEE/TSFC)

Access to symbolic representation of forms: automatic adjoints and derivatives, seamless switching between assembled and matrix-free, clever physics-based preconditioners, many other advantages

Intended to offer ”good enough” performance for many science applications (prototyping atmospheric dynamical cores is initial target application)
Example Code: $\mathcal{H}^1$ Helmholtz (in Firedrake, Themis and FEniCS very similar)

```python
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