Higher-order Structure-Preserving Finite Elements for Atmospheric Dynamical Cores

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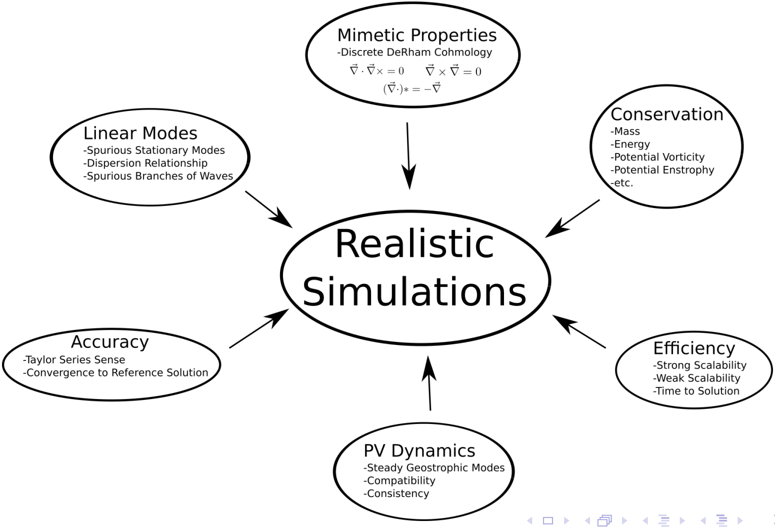
Introduction

(Incomplete) List of Desirable Model Properties



Incomplete History of Structure-Preserving Schemes for Atmospheric Models

- **The Beginning**: Arakawa and Lamb 1981, Sadourney 1975
- **Mimetic Finite Differences**: Ringler et. al 2010; Thuburn et. al 2012, 2014, many others
- **Mimetic Finite Elements**: Cotter et. al 2012,2013; McRae et. al 2014, Thuburn + Cotter 2015, many others
- **Hamiltonian Methods**: Salmon 2004,2005,2007; Sommer+Nevir 2009; Gassmann 2008,2013; Dubos et. al 2015; Tort et. al 2015, many others

What is structure-preservation?

1. **Mimetic Discretization**: curl-free pressure gradients, discrete product rules, discrete deRham cohomology, etc.

$$\vec{\nabla} \times \vec{\nabla} = 0$$

$$\vec{\nabla} \cdot \vec{\nabla} \times = 0$$

$$(\vec{\nabla} \cdot)^* = -\vec{\nabla}$$

2. **Quasi-Hamiltonian system**: conserves mass, total energy and possibly other invariants

$$\frac{d\mathcal{H}}{dt} = 0$$

$$\frac{d\mathcal{C}}{dt} = 0$$

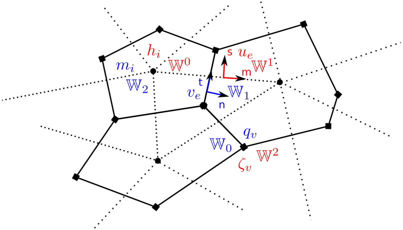
Mimetic Discretizations

General Formulation for Mimetic Discretizations: Primal-Dual Double deRham Complex (Staggered Grids)

$$
\begin{tikzcd}
\mathbb{W}_0 \arrow[r, "\vec{\nabla}^T"', "d"] \arrow[d, "*"] & \mathbb{W}_1 \arrow[r, "\vec{\nabla}\cdot"', "d"] \arrow[d, "*"] & \mathbb{W}_2 \arrow[d, "*"] \\
\mathbb{W}^2 & \mathbb{W}^1 \arrow[l, "\vec{\nabla}\times", "d"'] & \mathbb{W}^0 \arrow[l, "\vec{\nabla}", "d"']
\end{tikzcd}
$$

Outer Oriented Fluxes

Inner Oriented Circulations



$$\delta = *d*$$

$$\nabla^2 = d\delta + \delta d$$

$$\vec{\nabla}\cdot\vec{\nabla}\times = 0 = \vec{\nabla}\times\vec{\nabla}$$

$$\int_\Omega dW = \int_{d\Omega} W$$

$$dd = 0 = \delta\delta$$

General Formulation for Mimetic Discretizations: Primal deRham Complex

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

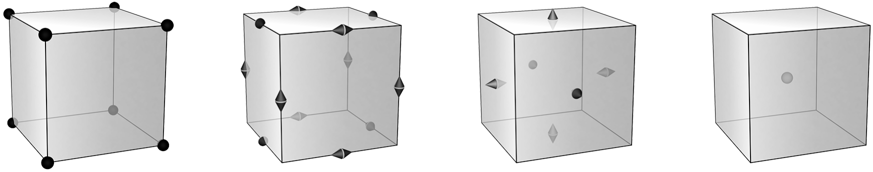
$$(da^k, b^{k+1}) = (a^k, \delta b^{k+1})$$

$$\delta = *d*$$

$$\nabla^2 = d\delta + \delta d$$

$$\vec{\nabla} \cdot \vec{\nabla} \times = 0 = \vec{\nabla} \times \vec{\nabla}$$

$$dd = 0 = \delta\delta$$



$\mathbb{W}_0$ $\mathbb{W}_1$ $\mathbb{W}_2$ $\mathbb{W}_3$

Hamiltonian

Non-Canonical Hamiltonian Dynamics

Evolution of an arbitrary functional $\mathcal{F} = \mathcal{F}[\vec{x}]$ is governed by:

$$\frac{d\mathcal{F}}{dt} = \{\frac{\delta \mathcal{F}}{\delta \vec{x}}, \frac{\delta \mathcal{H}}{\delta \vec{x}}\} \tag{1}$$

with Poisson bracket $\{,\}$ antisymmetric (also satisfies Jacobi):

$$\{\frac{\delta \mathcal{F}}{\delta \vec{x}}, \frac{\delta \mathcal{G}}{\delta \vec{x}}\} = -\{\frac{\delta \mathcal{G}}{\delta \vec{x}}, \frac{\delta \mathcal{F}}{\delta \vec{x}}\} \tag{2}$$

Also have Casimirs $\mathcal{C}$ that satisfy:

$$\{\frac{\delta \mathcal{F}}{\delta \vec{x}}, \frac{\delta \mathcal{C}}{\delta \vec{x}}\} = 0 \quad \forall \mathcal{F} \tag{3}$$

Neatly encapsulates conservation properties ($\mathcal{H}$ and $\mathcal{C}$).

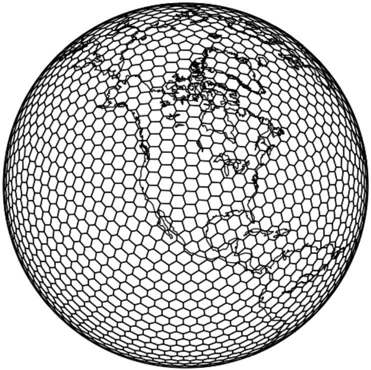
Recap: Mimetic + Hamiltonian = Structure-Preserving

- Fundamentally, structure-preserving schemes can be viewed as a combination of a **mimetic discretization method** plus a **hamiltonian formulation**
- Example: TRiSK Scheme (Primal-Dual ie Staggered Grid):

$$\frac{\partial \mathcal{F}}{\partial t} = \left(\frac{\delta \mathcal{A}}{m_i}, D_2 \frac{\delta \mathcal{B}}{u_e}\right)_{\mathbf{I}} + \left(\frac{\delta \mathcal{A}}{u_e}, \bar{D}_1 \frac{\delta \mathcal{B}}{m_i}\right)_{\mathbf{H}} + \left(\frac{\delta \mathcal{A}}{u_e}, \mathbf{Q} \frac{\delta \mathcal{B}}{u_e}\right)_{\mathbf{H}}$$

- D_2, $\bar{D}_1$ and $\mathbf{Q}$ are mimetic operators ($\mathbf{Q}$ is a little complicated)
- $(,)_{\mathbf{I}}$,$(,)_{\mathbf{J}}$,$(,)_{\mathbf{H}}$ are inner products (induced by Hodge stars)
- Scheme conserves mass, energy, potential vorticity; has curl-free pressure gradients, steady geostrophic modes, etc.

Dynamico



1. Primal-Dual: Mimetic finite differences (based on TRiSK scheme): C grid horizontal, Lorenz vertical
2. Icosahedral grid
3. Hydrostatic primitive equations: Lagrangian and mass-based vertical coordinates
4. Conserves mass, energy and entropy
5. See Dubos et. al 2015 for more information

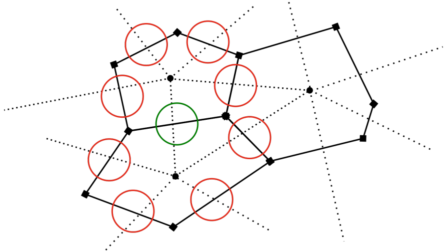
Reconstruction Operator (**W**) in TRiSK

$$\mathbf{W} = \sum_{e' \in ECP(e)} W_{e,e'}$$

$$\mathbf{W} = -\mathbf{W}^T$$

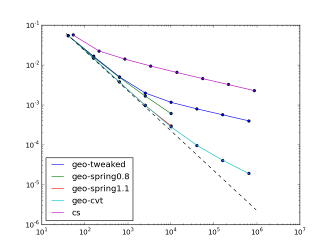
$$-\mathbf{R} D_2 = \bar{D}_2 \mathbf{W}$$

Given normal fluxes, reconstruct tangential fluxes
Satisfying: Steady geostrophic modes AND energy conservation AND accuracy

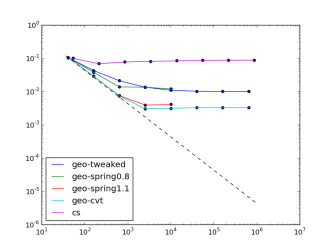


Issues with TRiSK

Operator Accuracy



L_2 for $\mathbf{W}$

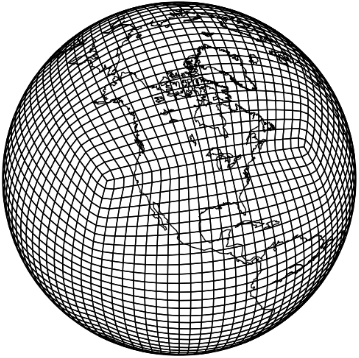


L_∞ for $\mathbf{W}$

Spurious Branches of Dispersion Relationship

Hexagonal grid means 3:1 ratio of wind to mass dofs (should be 2:1) $\rightarrow$ spurious branch of Rossby waves with unphysical behaviour

How do we fix them?



1. Fix spurious branches: Quadrilateral (cubed-sphere) grid, correct 2:1 ratio of dofs
2. Fix accuracy: Use Primal approach (mimetic Galerkin methods)
3. Keep the same equations and Hamiltonian structure
4. Keep the same mimetic and conservation properties

Mimetic Galerkin Discretization

Mimetic Galerkin Discretization

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

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

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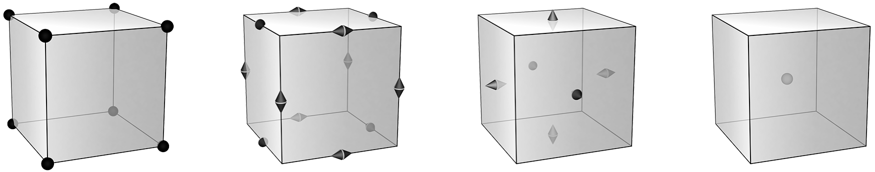


$\mathbb{W}_0$ $\mathbb{W}_1$ $\mathbb{W}_2$ $\mathbb{W}_3$

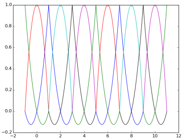
General Approach to Mimetic Galerkin Spaces

Mimetic Spaces

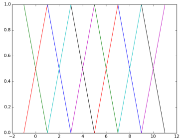
$$\text{Select 1D Spaces } \mathcal{A} \text{ and } \mathcal{B} \text{ such that } : \mathcal{A} \xrightarrow{\frac{d}{dx}} \mathcal{B} \tag{4}$$

- Use tensor products to extend to n-dimensions
- Works for ANY set of spaces $\mathcal{A}$ and $\mathcal{B}$ that satisfy this property (mimetic finite elements use P_n and $P_{DG,n-1}$)
- Mimetic spectral element, Mimetic isogeometric methods (B-splines) all fall under this framework
- Our (different) choices of $\mathcal{A}$ and $\mathcal{B}$ are guided by linear mode properties and coupling to physics/tracer transport
- See Hiemstra et. al 2014 (and references therein)

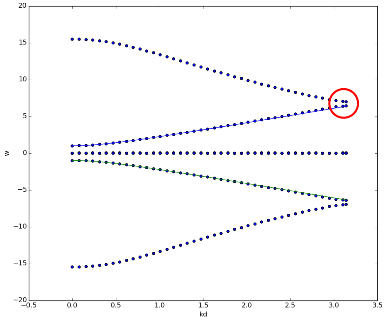
$P_2 - P_{1,DG}$ Dispersion Relationship



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



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

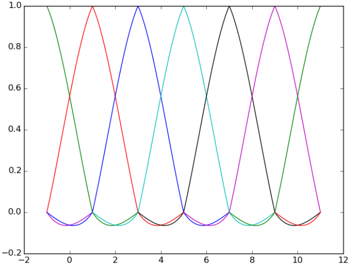


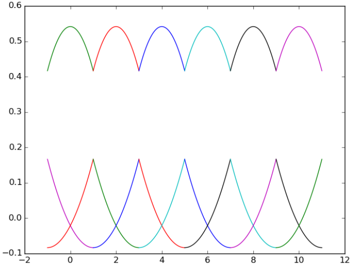
Inertia-Gravity Wave Dispersion Relationship (1D)

Multiple dofs per element $\rightarrow$ breaks translational invariance $\rightarrow$ spectral gaps

We have developed an alternative: mimetic Galerkin differences

Mimetic Galerkin Differences: Basis





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

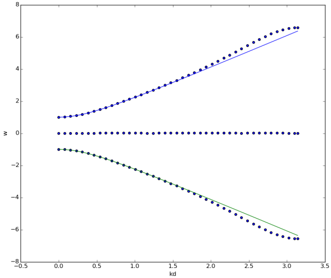
$\mathcal{B} = L_2$ Space (1D)

Single degree of freedom per geometric entity (physics coupling)

Higher order by larger stencils (less local)

3rd Order Elements

Mimetic Galerkin Differences- Dispersion



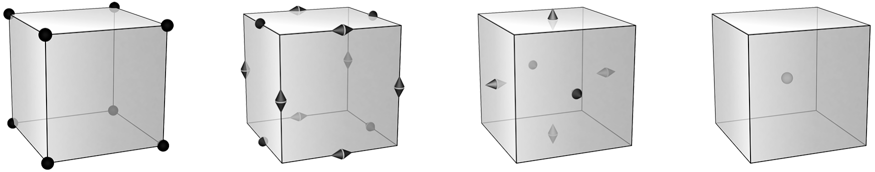
Inertia-Gravity Wave Dispersion Relationship (1D) for 3rd Order Elements

Spectral gap is gone

Can show that dispersion relation is $O(2n)$ where n is the order

More details in a forthcoming paper

Overview of 3D Spaces

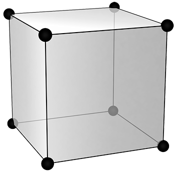


$\mathbb{W}_0$ $\mathbb{W}_1$ $\mathbb{W}_2$ $\mathbb{W}_3$

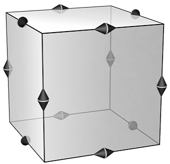
$$\mathbb{W}_0 \xrightarrow{\vec{\nabla}} \mathbb{W}_1 \xrightarrow{\vec{\nabla}\times} \mathbb{W}_2 \xrightarrow{\vec{\nabla}\cdot} \mathbb{W}_3$$

$\mathbb{W}_0 = \mathcal{A} \otimes \mathcal{A} \otimes \mathcal{A} = H_1 =$ Continuous Galerkin
$\mathbb{W}_1 = (\mathcal{B} \otimes \mathcal{A} \otimes \mathcal{A})\hat{i} + \dots = H(curl) =$ Nedelec
$\mathbb{W}_2 = (\mathcal{A} \otimes \mathcal{B} \otimes \mathcal{B})\hat{i} + \dots = H(div) =$ Raviart-Thomas
$\mathbb{W}_3 = \mathcal{B} \otimes \mathcal{B} \otimes \mathcal{B} = L_2 =$ Discontinuous Galerkin

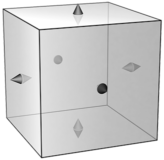
Grid Staggering for HPE



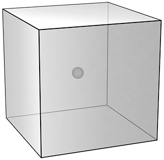
$\mathbb{W}_0$
Θ
Differential Geometry



$\mathbb{W}_1$
$\vec{\zeta}$



$\mathbb{W}_2$
$\vec{v},\vec{u},W,\Theta$
CP Grid



$\mathbb{W}_3$
μ,Θ,δ
L Grid

Follows from differential geometry and Tonti diagram
Galerkin Version of a C Grid
Question: Where should Θ live?

Hamiltonian Formulation

Poisson Brackets (Lagrangian Vertical Coordinate)

Poisson Brackets

From Dubos and Tort 2014, evolution of $\mathcal{F}[\vec{x}] = \mathcal{F}[\mu, \vec{v}, \Theta, z]$ is

$$\frac{d\mathcal{F}}{dt} = \{\frac{\delta\mathcal{F}}{\delta\vec{x}}, \frac{\delta\mathcal{H}}{\delta\vec{x}}\}sw + \{\frac{\delta\mathcal{F}}{\delta\vec{x}}, \frac{\delta\mathcal{H}}{\delta\vec{x}}\}_\Theta + \langle\frac{\delta\mathcal{F}}{\delta z}\frac{\partial z}{\partial t}\rangle \tag{5}$$

$$\{\frac{\delta\mathcal{F}}{\delta\vec{x}}, \frac{\delta\mathcal{H}}{\delta\vec{x}}\}sw = \langle\frac{\delta\mathcal{H}}{\delta\vec{v}} \cdot \vec{\nabla}\frac{\delta\mathcal{F}}{\delta\mu} - \frac{\delta\mathcal{H}}{\delta\vec{v}} \cdot \vec{\nabla}\frac{\delta\mathcal{F}}{\delta\mu}\rangle + \langle\frac{\vec{\nabla}\times\vec{v}}{\mu} \cdot (\frac{\delta\mathcal{F}}{\delta\vec{v}} \times \frac{\delta\mathcal{H}}{\delta\vec{v}})\rangle \tag{6}$$

$$\{\frac{\delta\mathcal{F}}{\delta\vec{x}}, \frac{\delta\mathcal{H}}{\delta\vec{x}}\}_\Theta = \langle\theta(\frac{\delta\mathcal{H}}{\delta\vec{v}} \cdot \vec{\nabla}\frac{\delta\mathcal{F}}{\delta\Theta} - \frac{\delta\mathcal{H}}{\delta\vec{v}} \cdot \vec{\nabla}\frac{\delta\mathcal{F}}{\delta\Theta})\rangle \tag{7}$$

where μ is the pseudo-density, $\vec{v} = \vec{u} - \vec{R}$ is the absolute (covariant) velocity, $\Theta = \mu\theta$ is the mass-weighted potential temperature and z is the height.

Equations of Motion: Lagrangian Vertical Coordinate

Equations of Motion

Choose $\mathcal{F} = \int \hat{\mu}$ (or $\int \hat{v} / \int \hat{\Theta} / \int \hat{z}$) to get:

$$\int \hat{\mu} \left(\frac{\partial \mu}{\partial t} + \vec{\nabla} \cdot \left(\frac{\delta \mathcal{H}}{\delta \vec{v}} \right) \right) = 0 \tag{8}$$

$$\int \hat{\Theta} \left(\frac{\partial \Theta}{\partial t} + \vec{\nabla} \cdot \left(\theta \frac{\delta \mathcal{H}}{\delta \vec{v}} \right) \right) = 0 \tag{9}$$

$$\int \hat{v} \left(\frac{\partial \vec{v}}{\partial t} + \frac{\zeta_v}{\mu} \times \frac{\delta \mathcal{H}}{\delta \vec{v}} + \theta \vec{\nabla} \left(\frac{\delta \mathcal{H}}{\delta \Theta} \right) + \vec{\nabla} \left(\frac{\delta \mathcal{H}}{\delta \mu} \right) \right) = 0 \tag{10}$$

$$\int \hat{z} \frac{\delta \mathcal{H}}{\delta z} = \int \hat{z} \left(g\mu + \frac{\partial p}{\partial \eta} \right) = 0 \tag{11}$$

Note that these are ALL 2D except for hydrostatic balance (11)

Hamiltonian (Lagrangian Vertical Coordinate)

Hamiltonian and Functional Derivatives

$$\mathcal{H} = \mathcal{H}[\mu, \vec{v}, \Theta, z] = \int \mu(\frac{\vec{u} \cdot \vec{u}}{2} + U(\frac{1}{\mu}\frac{\partial z}{\partial \eta}, \frac{\Theta}{\mu}) + gz) \quad (12)$$

$$\int \hat{v} \frac{\delta \mathcal{H}}{\delta \vec{v}} = \int \hat{v} \, (\mu \vec{u}) \quad (13)$$

$$\int \hat{\mu} \frac{\delta \mathcal{H}}{\delta \mu} = \int \hat{\mu} \left(\frac{\vec{u} \cdot \vec{u}}{2} + gz \right) \quad (14)$$

$$\int \hat{\Theta} \frac{\delta \mathcal{H}}{\delta \Theta} = \int \hat{\Theta} \frac{\partial U}{\partial \theta} = \int \hat{\Theta} \pi \quad (15)$$

$$\int \hat{z} \frac{\delta \mathcal{H}}{\delta z} = \int \hat{z} \left(g\mu + \frac{\partial p}{\partial \eta} \right) \quad (16)$$

Conservation

Energy

- Arises purely from anti-symmetry of the brackets PLUS $\frac{\delta \mathcal{H}}{\delta z} = 0$
- Mimetic Galerkin methods automatically ensure an anti-symmetric bracket
- Works for ANY choice of $\mathcal{H}$
- Something similar can be done with a mass-based vertical coordinate, although it is slightly more complicated

Mass, Potential Vorticity and Entropy

- These are Casimirs
- Can show that this discretization also conserves them

Remaining Issues and Questions

Hydrostatic Balance

1. Dynamico: Column-wise direct solution
2. Can this also be done with Galerkin approach?

Grid Staggering: Placement of Θ

1. Dynamico: Lorenz staggering (Θ and μ are collocated)
2. Galerkin Equivalent: $\mu,\Theta \in \mathbb{W}_3$ (Admits a spurious computational mode in the vertical)
3. Charney-Phillips: $\Theta \in \mathbb{W}_{2,vert}$ (Avoids computational mode, complicates formulation)
4. Differential Geometry: Θ is a 0-form $\rightarrow \Theta \in \mathbb{W}_0$ (Excessive horizontal averaging $\rightarrow$ computational mode/poor dispersion properties?)

Summary and Conclusions

Summary and Conclusions

Summary

1. There is a general, effective procedure for devising mimetic, conservative numerical schemes:
2. **Mimetic discretizations + Hamiltonian formulation**

Future Work

1. Computational efficiency: preconditioning/solvers, matrix assembly
2. Mass-based vertical coordinate
3. Nonhydrostatic equations
4. Past Inivscid, Adiabatic Dry Dynamics: Subgrid Turbulence, Moisture, Tracers, Physics Coupling