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

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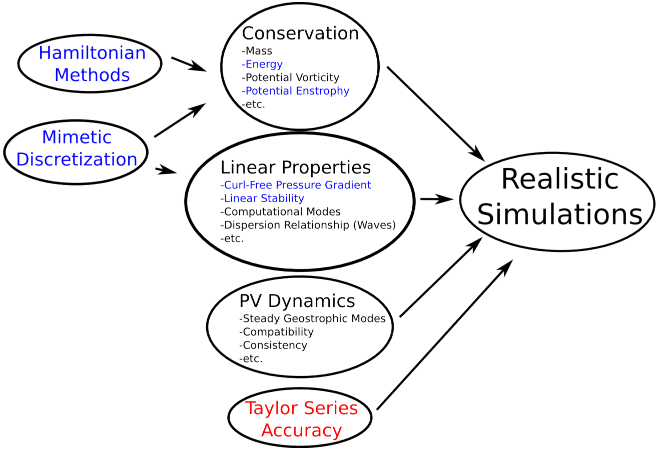
Introduction

Elements of Dynamical Core Design



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 2012,201; McRae et. al 2014, many others
- Hamiltonian: Salmon 2004,2005,2007; Sommer+Nevir 2009; Gassmann 2008,2013; Dubos et. al 2015; Tort et. al 2015, many others
- Fundamentally, structure-preserving schemes can be viewed as a combination of a **mimetic discretization method** plus a **hamiltonian formulation**

What is structure-preservation?

1. Discrete deRham cohomology (mimetic discretization)

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

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

2. Quasi-Hamiltonian system (conserves total energy, and possibly other invariants)

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

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

General Formulation for Mimetic Discretizations: Primal-Dual Double deRham Complex

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

$$\delta = *d*$$

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

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

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

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

General Formulation for Mimetic Discretizations: Primal deRham Complex

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

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

$$\delta = *d*$$

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

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Non-Canonical Hamiltonian Dynamics

Poisson Brackets

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):

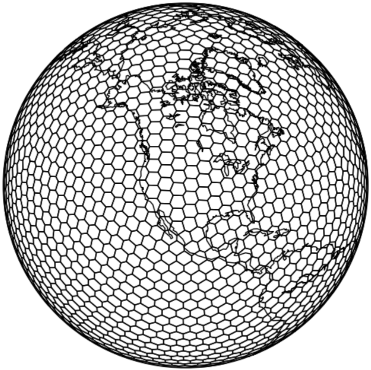
$$\{\frac{\delta \mathcal{F}}{\delta \vec{x}}, \frac{\delta \mathcal{G}}{\delta \vec{x}}\} = -\{\frac{\delta \mathcal{G}}{\delta \vec{x}}, \frac{\delta \mathcal{F}}{\delta \vec{x}}\} \tag{2}$$

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 $\mathcal{C}$).

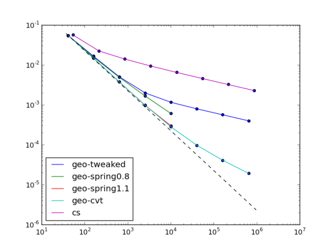
Dynamico



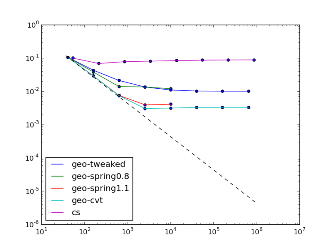
1. Primal-Dual: Mimetic finite differences (based on TRiSK scheme): C grid horizontal, Lorenz vertical
2. Icosahedral grid
3. Hydrostatic primitive equations: Lagrangian and mass-based vertical coordinates
4. Conserves mass, energy and entropy
5. See Dubos et. al 2015 for more information

Issues in Dynamico

Operator Accuracy



L_2 for $\mathbf{W}$

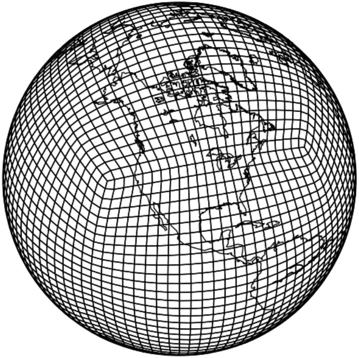


L_∞ for $\mathbf{W}$

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

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

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

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

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

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

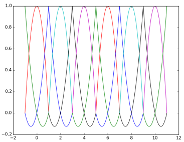
General Approach to Mimetic Galerkin Spaces

Mimetic Spaces

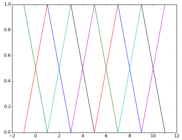
$$\text{Select 1D Spaces } \mathcal{A} \text{ and } \mathcal{B} \text{ such that } : \mathcal{A} \xrightarrow{\frac{d}{dx}} \mathcal{B} \tag{4}$$

- 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)

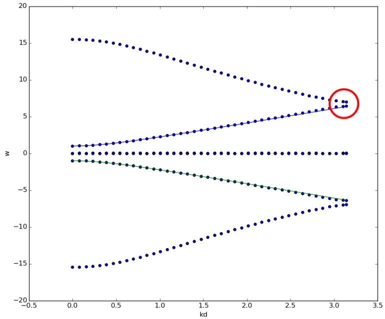
$P_2 - P_{1,DG}$ Dispersion Relationship



$\mathcal{A} = H_1$ Space



$\mathcal{B} = L_2$ Space

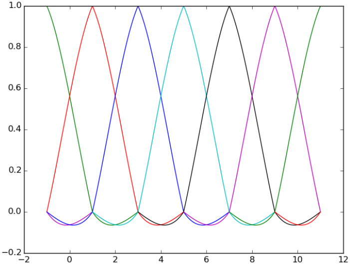


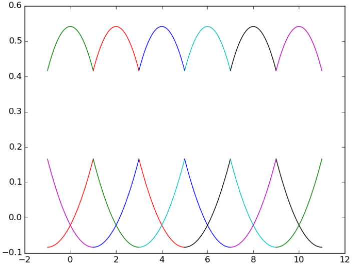
Inertia-Gravity Wave Dispersion Relationship (1D)

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

We have developed an alternative: mimetic Galerkin differences

Mimetic Galerkin Differences: Basis





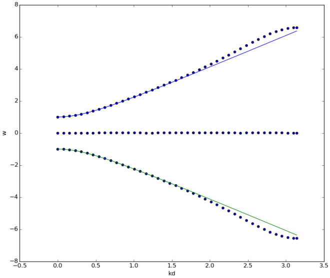
$\mathcal{A} = H_1$ Space

$\mathcal{B} = L_2$ Space

Single degree of freedom per geometric entity (physics coupling)

Higher order by larger stencils (less local)

Mimetic Galerkin Differences- Dispersion



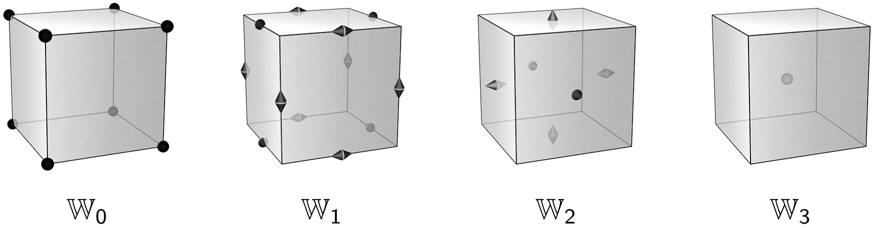
Inertia-Gravity Wave Dispersion Relationship (1D)

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



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

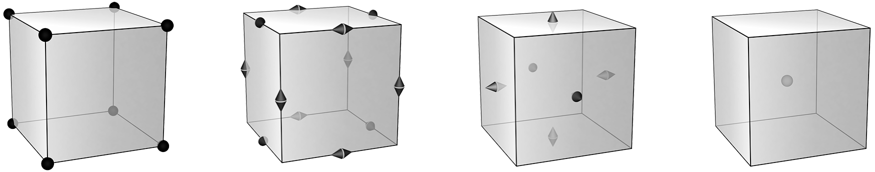
$\mathbb{W}_0 = \mathcal{A} \otimes \mathcal{A} \otimes \mathcal{A} = H_1 =$ Continuous Galerkin

$\mathbb{W}_1 = (\mathcal{B} \otimes \mathcal{A} \otimes \mathcal{A})\hat{i} + \dots = H(curl) =$ 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



$\mathbb{W}_0$	$\mathbb{W}_1$	$\mathbb{W}_2$	$\mathbb{W}_3$
ψ,Θ	$\vec{\zeta}$	$\vec{v}$,$\vec{u}$,W,Θ	μ,Θ,δ,χ
Differential Geometry		CP Grid	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, $\Theta = \theta\mu$ 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 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: μ,$\Theta \in \mathbb{W}_3$ (Admits a spurious computational mode in the vertical)
3. Charney-Phillips: $\Theta \in \mathbb{W}_{2,vert}$ (Avoids computational mode, more difficult to obtain conservation, 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 numerical schemes that mimic important characteristics of the real atmosphere
2. **Combine mimetic discretizations with a Hamiltonian formulation**

Future Work

1. Computational efficiency: preconditioning, assembly, etc.
2. Mass-based vertical coordinate
3. Non-hydrostatic equations
4. Subgrid Turbulence, Moisture, Tracers, Physics Coupling