A Hydrostatic Dynamical Core using Higher-Order Structure-Preserving Finite Elements

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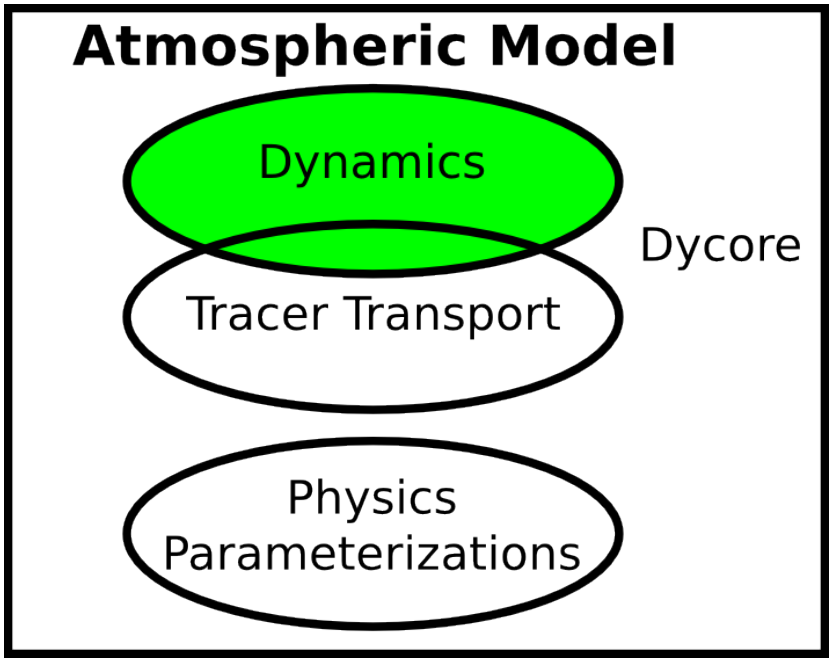
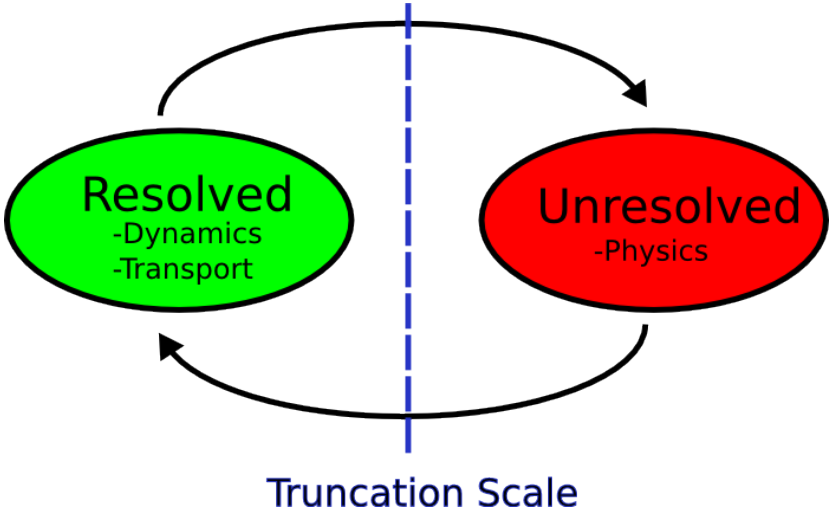
Introduction

Broad Research Overview: Dynamical Cores

1. Solve the Euler equations for a rotating fluid
2. Limited computational resources $\rightarrow$ truncation scale
3. Dynamical core: "resolved" adiabatic, inviscid part of the flow

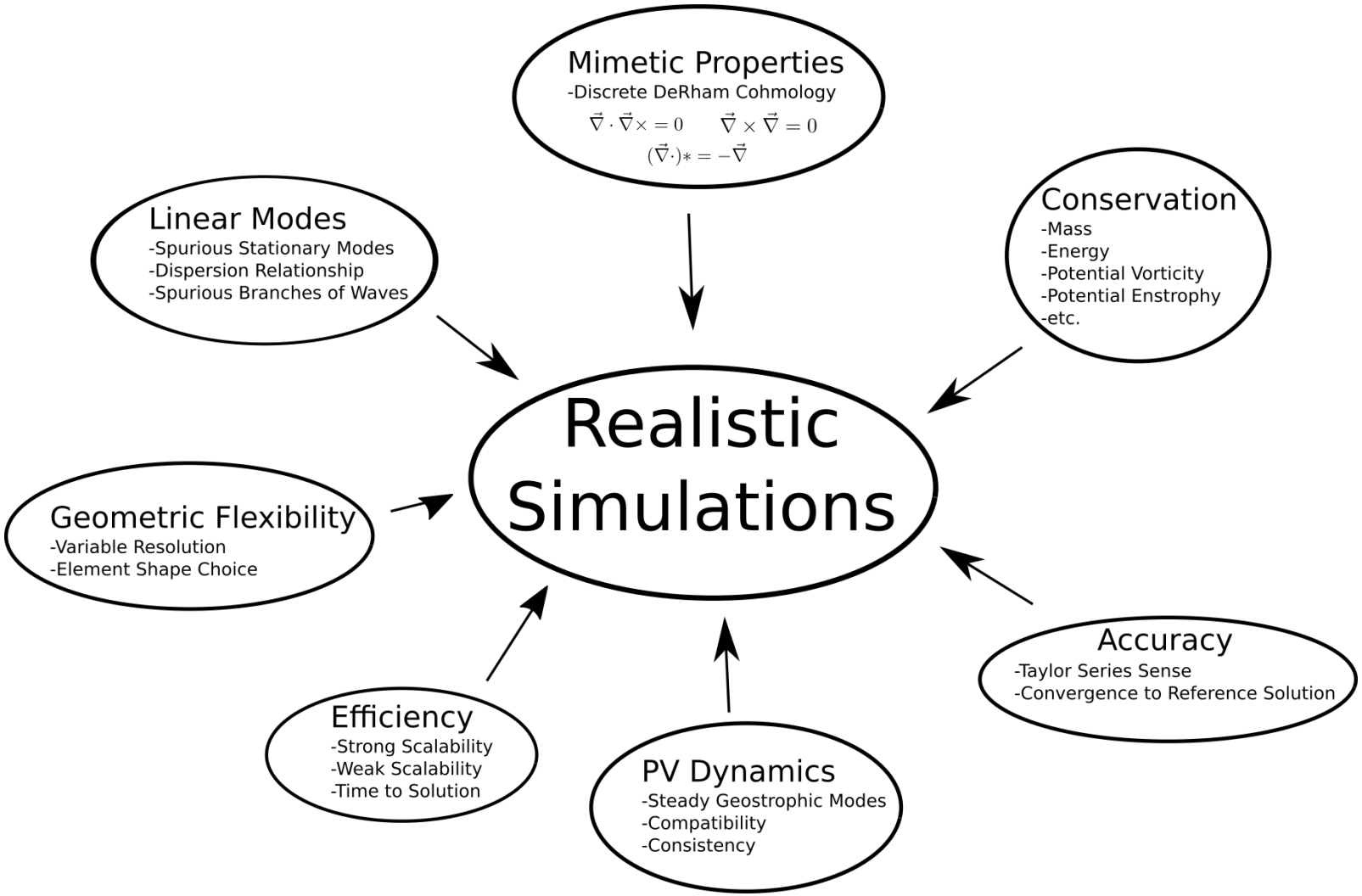




Key Principle of Numerical Modeling

1. Not solving arbitrary PDEs- physical system
2. No analytic solutions
3. Differential equations $\rightarrow$ algebraic equations
4. **Do algebraic solutions have the same properties as the differential (true) solutions?**

(Incomplete) List of Desirable Model Properties (NLSWE)



Motivating science questions

1. For canonical, finite-dimensional Hamiltonian systems, structure-preserving numerics are essential to obtain correct long-term statistical behavior
2. The equations of (moist) adiabatic, inviscid atmospheric dynamics are a non-canonical, infinite-dimensional Hamiltonian system
3. To what extent does (1) hold for models of the atmosphere, given (2), especially since the real atmosphere has forcing and dissipation that makes it non-Hamiltonian?
4. **Studying these questions requires a structure-preserving atmospheric model!**

Structure Preservation

What is structure-preservation?

Obtaining these properties

1. **Quasi-Hamiltonian Formulation**: Easily expresses conservation of mass, total energy and possibly other invariants

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

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

2. **Mimetic Discretization**: Discrete analogues of vector calculus identities (such as curl-free vorticity, div and grad are adjoints, etc.)

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

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

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

General Formulation for Mimetic Discretizations: Primal deRham Complex (Finite Element Type Methods)

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

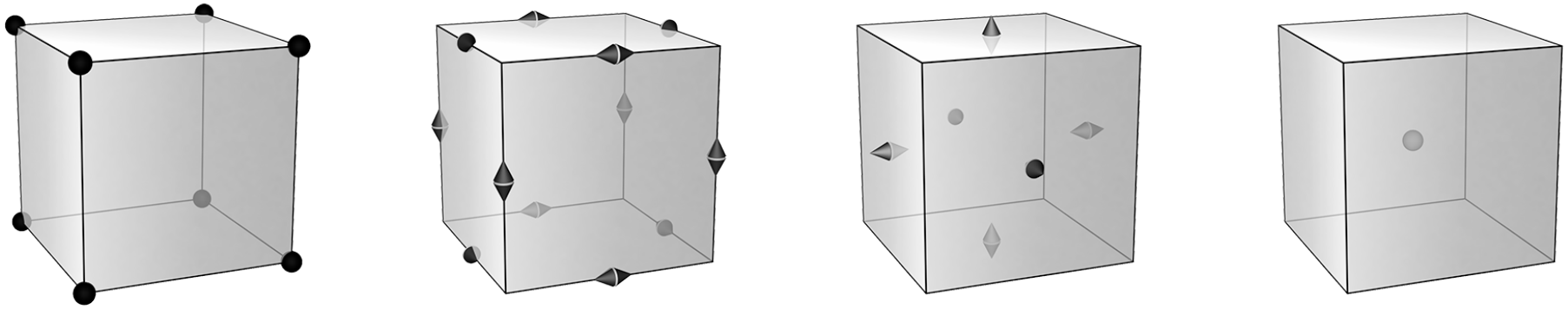
$$(da^k, b^{k+1}) = (a^k, \delta b^{k+1})$$

$$\delta = *d*$$

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

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

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



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

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):

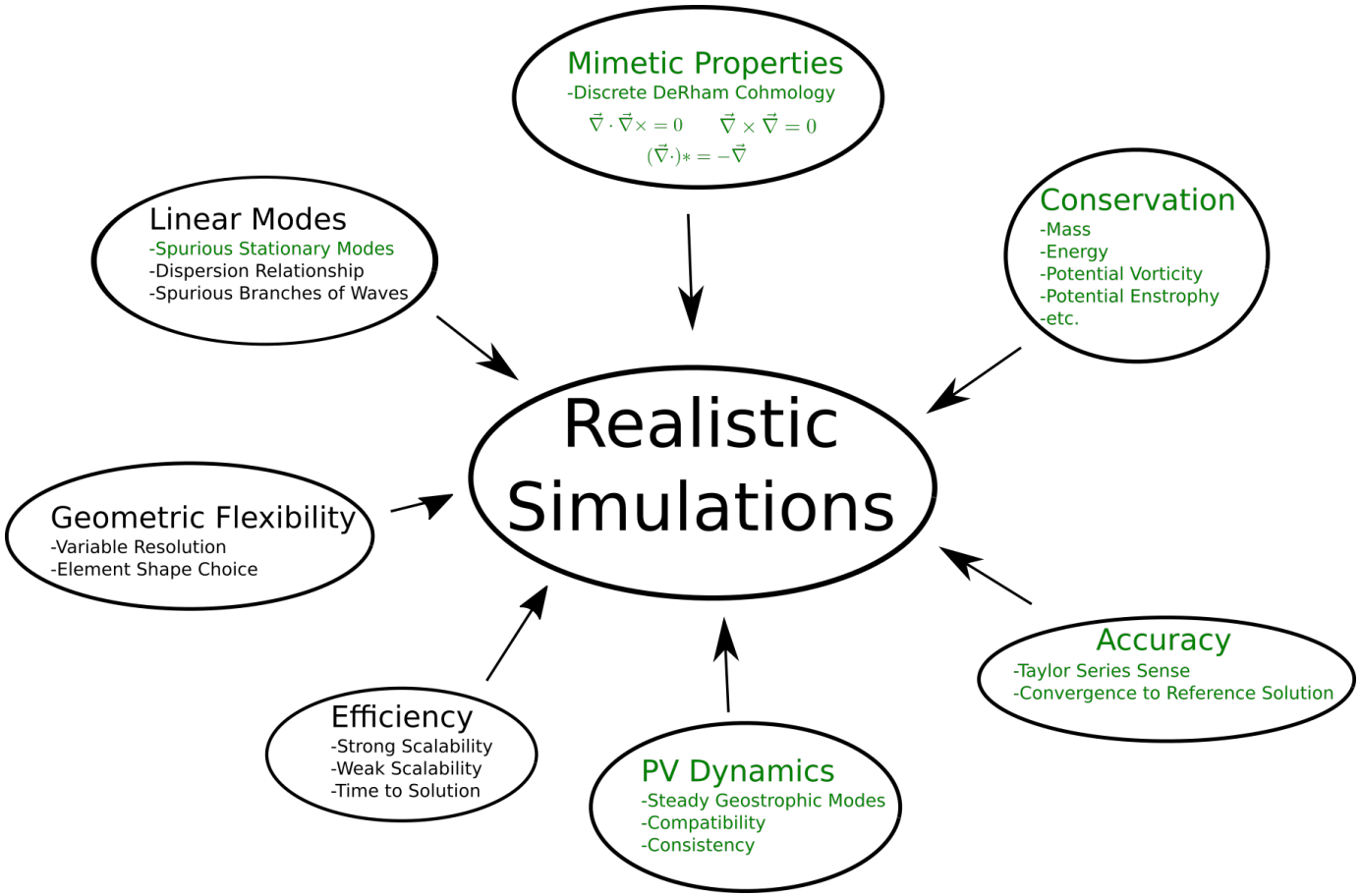
$$\{\frac{\delta\mathcal{F}}{\delta\vec{x}}, \frac{\delta\mathcal{G}}{\delta\vec{x}}\} = -\{\frac{\delta\mathcal{G}}{\delta\vec{x}}, \frac{\delta\mathcal{F}}{\delta\vec{x}}\} \tag{2}$$

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

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

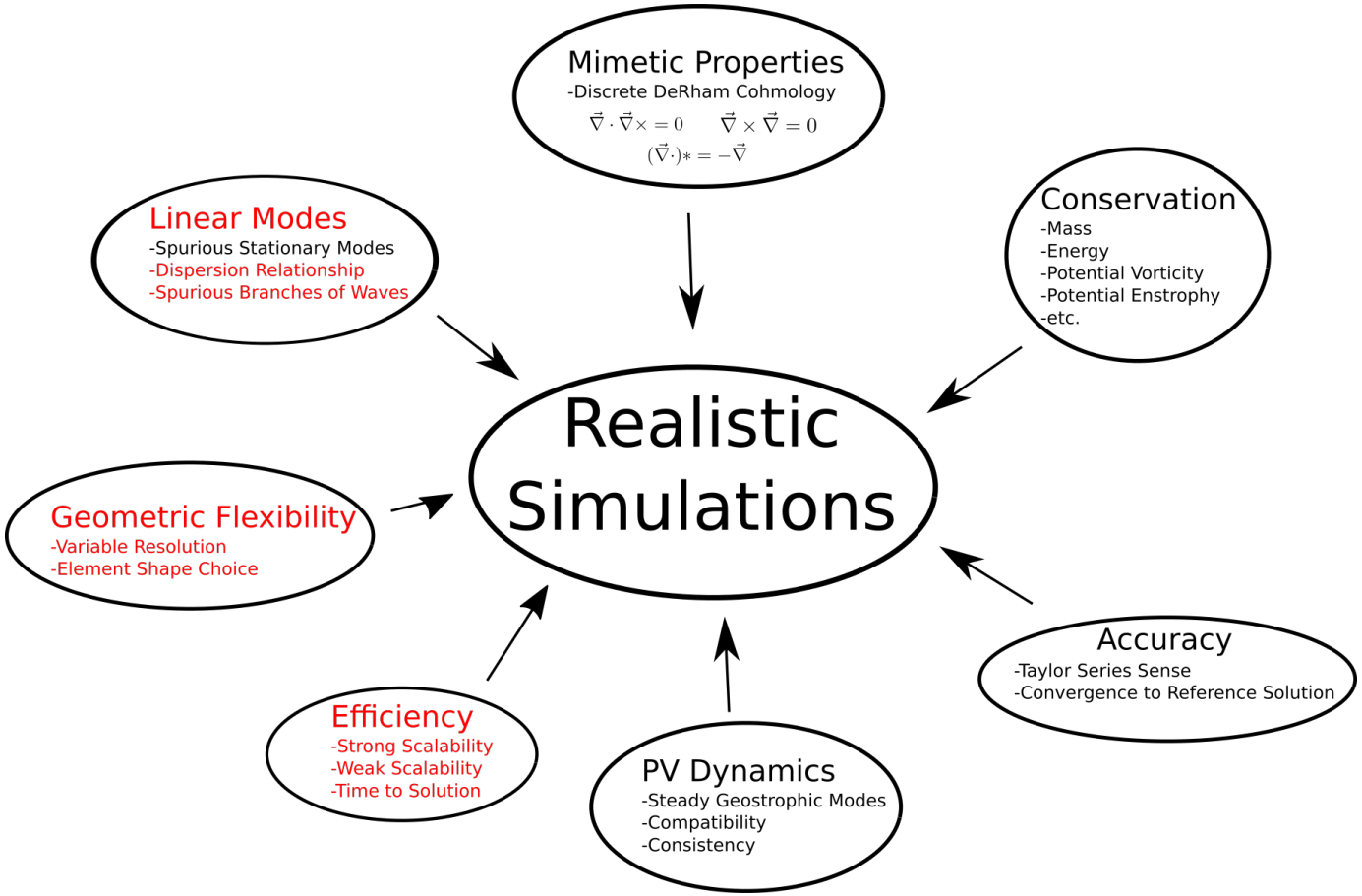
Neatly encapsulates conservation properties ($\mathcal{H}$ and $\mathcal{C}$).

What properties do we get?



There are MANY choices of spaces that give these properties: key point is the deRham complex

What properties are still lacking?



These are a function of the specific choice of spaces

Tensor Product Mimetic Galerkin Methods

Tensor Product Mimetic Galerkin Spaces

Tensor Product Mimetic Galerkin Spaces

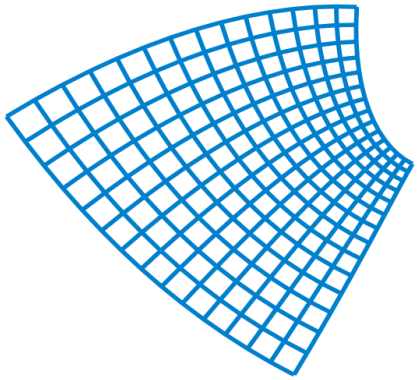
$$\text{Select 1D Spaces } \mathcal{A} \text{ and } \mathcal{B} \text{ such that } : \mathcal{A} \xrightarrow{\frac{d}{dx}} \mathcal{B} \tag{4}$$

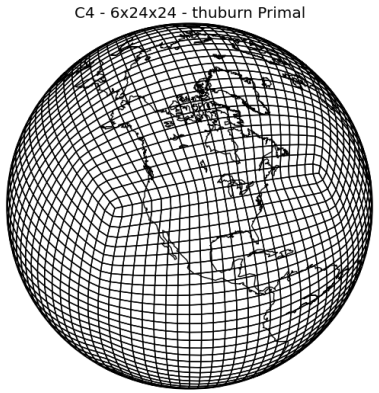
- Use tensor products to extend to n-dimensions
- Works for ANY set of spaces $\mathcal{A}$ and $\mathcal{B}$ that satisfy this property (mimetic finite elements use P_n and $P_{DG,n-1}$)
- Mimetic spectral element, Mimetic isogeometric methods (B-splines) all fall under this framework
- Our (different) 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)

How do we get the remaining properties?

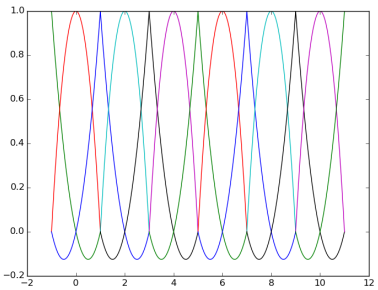
Tensor Product Mimetic Galerkin Methods on Structured Grids

1. **Tensor product + structured grids**: efficiency (for a method with non-diagonal mass matrices)
2. **Quadrilateral grids**- no spurious wave branches
3. **Key: What about dispersion relationships?**
4. **Also: What about geometric flexibility?**

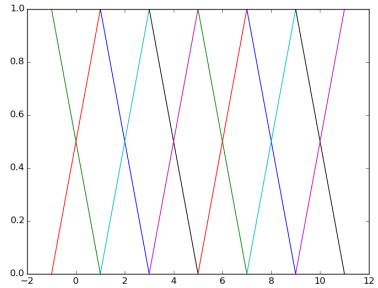




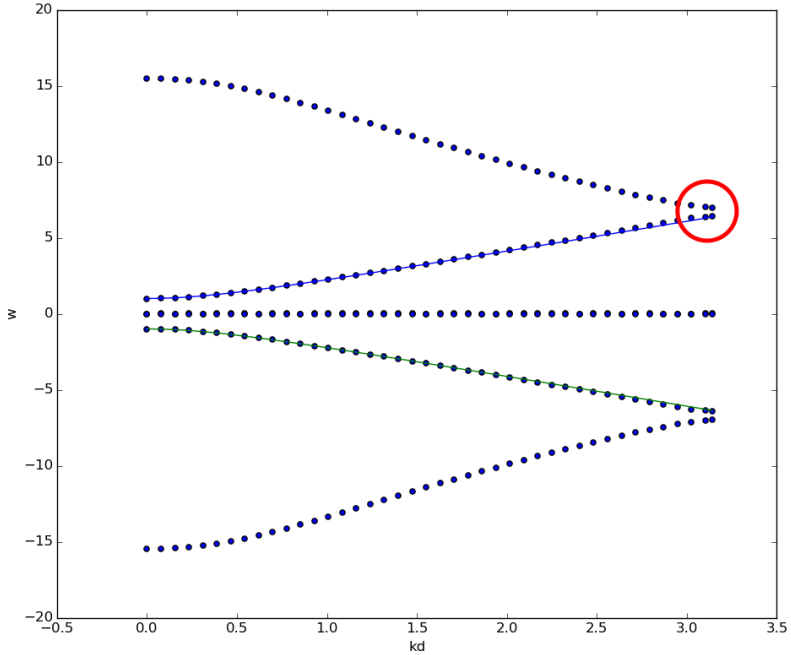
$P_2 - P_{1,DG}$ Dispersion Relationship



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



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

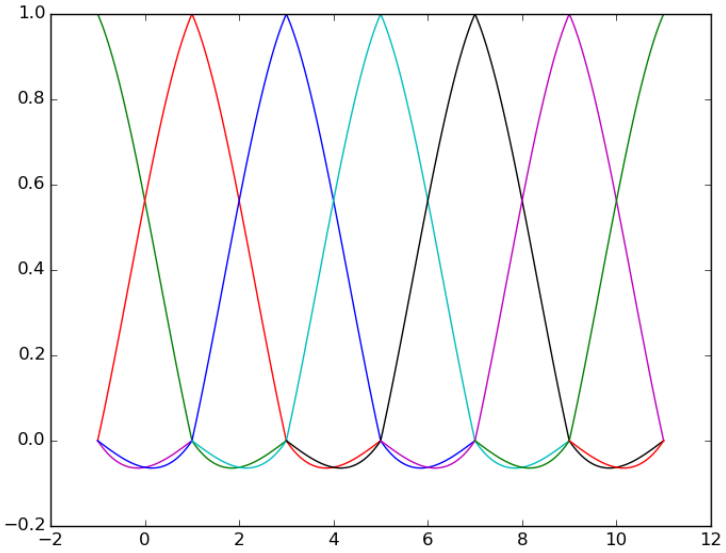


Inertia-Gravity Wave Dispersion Relationship (1D)

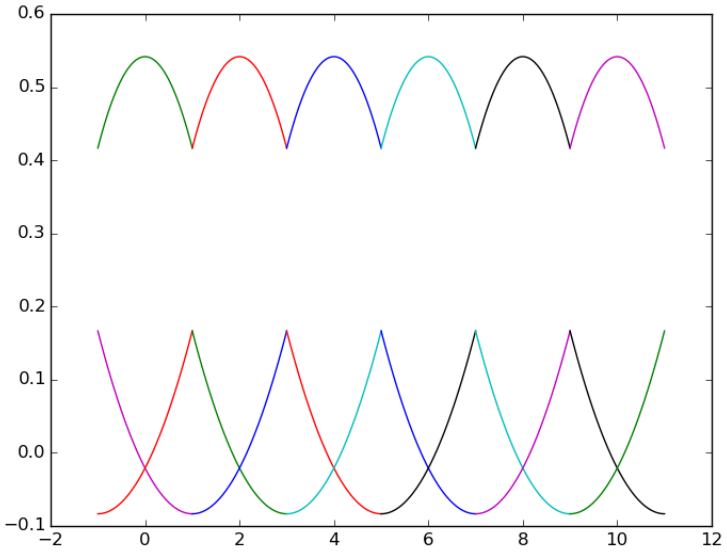
Multiple dofs per element $\rightarrow$ breaks translational invariance $\rightarrow$ spectral gaps

We have developed an alternative: mimetic Galerkin differences

Mimetic Galerkin Differences: Basis (3rd Order)



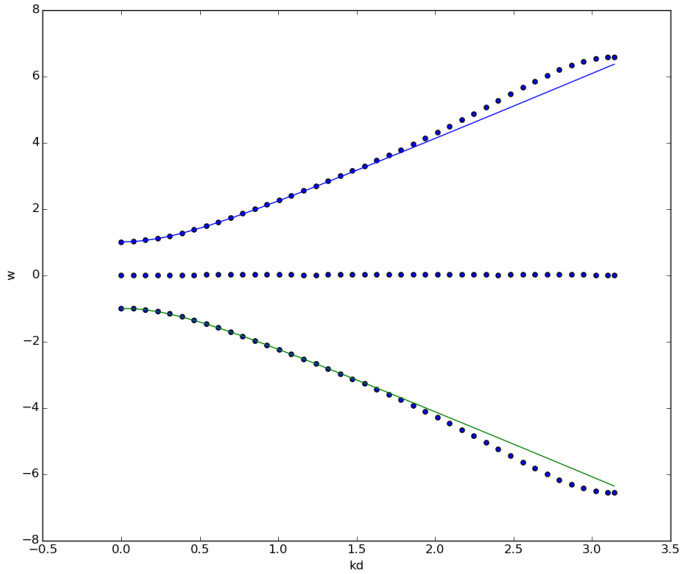
$\mathcal{A} = H_1$ Space (1D)



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

Single degree of freedom per geometric entity (physics coupling)
Higher order by larger stencils (less local, efficiency concerns)
Shown for 3rd Order Elements (works for arbitrary order)

Mimetic Galerkin Differences- Dispersion



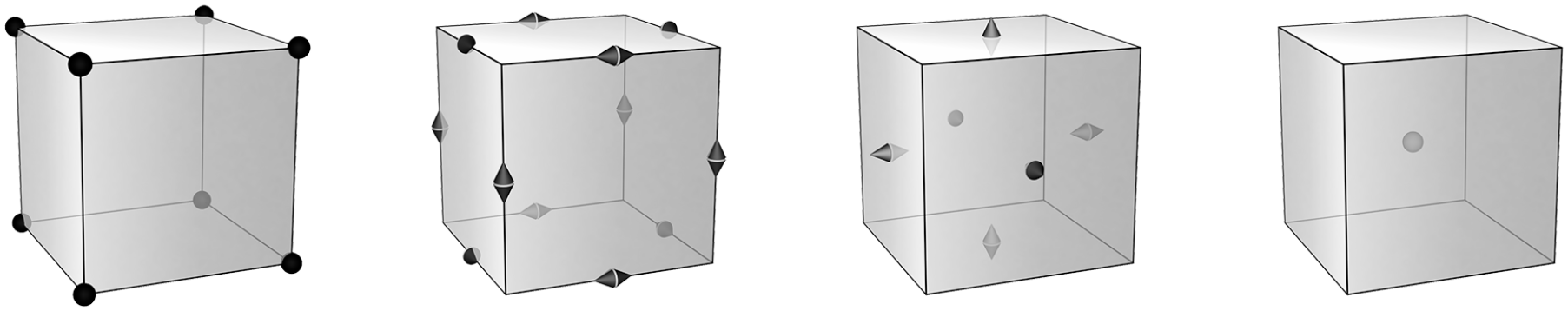
Inertia-Gravity Wave Dispersion Relationship (1D) for 3rd Order Elements

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

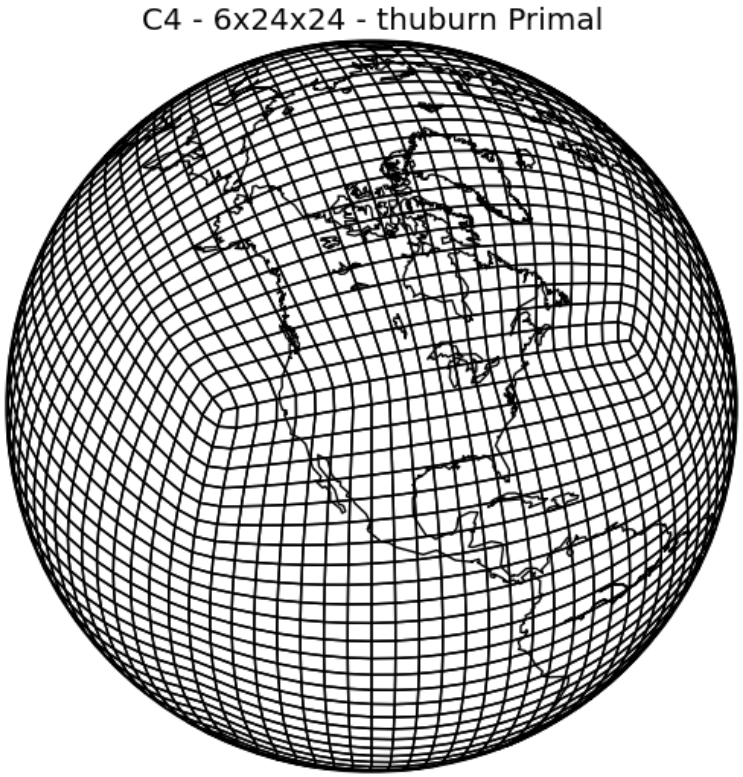


$\mathbb{W}_0$ $\mathbb{W}_1$ $\mathbb{W}_2$ $\mathbb{W}_3$

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

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

Dynamico-FE



1. Hydrostatic primitive equations
2. Mimetic Galerkin discretization
3. Hamiltonian formulation
4. Lagrangian and Mass-Based Vertical Coordinates
5. Cubed-Sphere Grid
6. Conserves mass, entropy and total energy
7. Has the complete set of properties discussed at the beginning

Current Status

Current Status of Dynamico-FE

1. Multilayer Ripa Equations with full set of desired properties
2. Very close to an HPE model in lagrangian vertical coordinates

Themis*

1. Software library for tensor-product Galerkin methods on (block-)structured grids with arbitrary geometric mappings
2. Built on top of PETSc; written in Python and C
3. Parallelism through MPI

*-Available online at `https://bitbucket.org/chris_eldred/themis`

Future Work, Summary and Conclusions

Future Work

Future Work

1. Computational efficiency: preconditioning, solvers, matrix-free
2. Mass-based vertical coordinate
3. Nonhydrostatic equations
4. Past Inivscid, Adiabatic Dry Dynamics: Subgrid Turbulence, Moisture, Tracers, Physics Coupling
5. Time stepping and 4D formulations
6. Removal of other approximations: Deep-atmosphere/quasi-hydrostatic, non-traditional, non-spherical, vertical and latitudinal variation of gravity

Summary and Conclusions

Summary

1. Developing a structure-preserving atmospheric dynamical core: Dynamico-FE
2. Use tensor-product Galerkin methods on structured grids: Obtain almost all the desired properties
3. Mimetic Galerkin Differences: Fixes dispersion issues

Conclusions

1. **Mimetic discretizations + Hamiltonian formulation** = Structure-Preservation = (Most) Desired Properties
2. **Many** choices of mimetic discretization, select the one that gets the other properties

Additional Slides

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

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

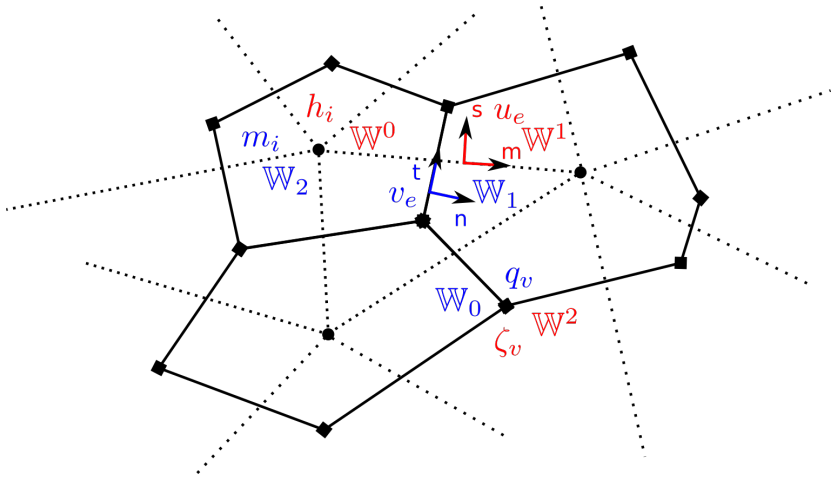
Outer Oriented Fluxes

Inner Oriented Circulations

$$\delta = *d*$$

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

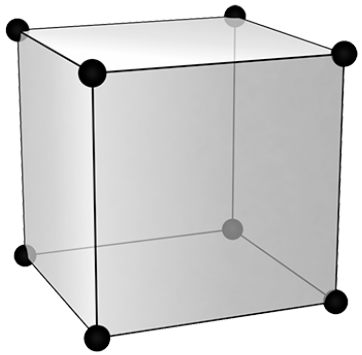
$$\vec{\nabla} \cdot \vec{\nabla}\times = 0 = \vec{\nabla} \times \vec{\nabla}$$



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

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

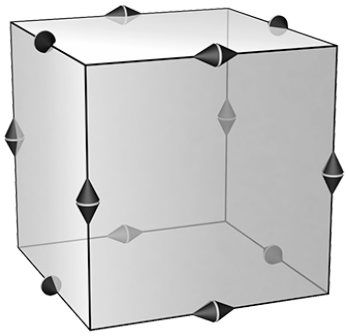
Grid Staggering for HPE



$\mathbb{W}_0$

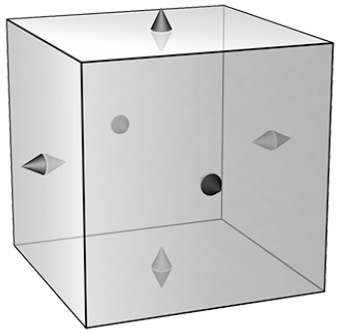
Θ

Differential Geometry



$\mathbb{W}_1$

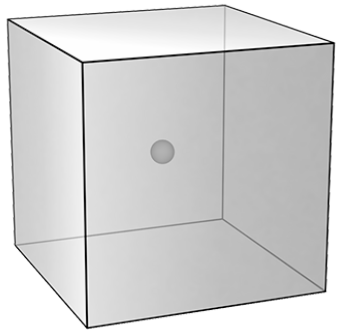
$\vec{\zeta}$



$\mathbb{W}_2$

$\vec{v}, \vec{u}, W, \Theta$

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?

Grid Staggering: Θ, p, θ and z

Grid Staggering: Placement of Θ

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

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 (8)

Hamiltonian (Lagrangian Vertical Coordinate)

Hamiltonian and Functional Derivatives

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

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

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

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

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

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

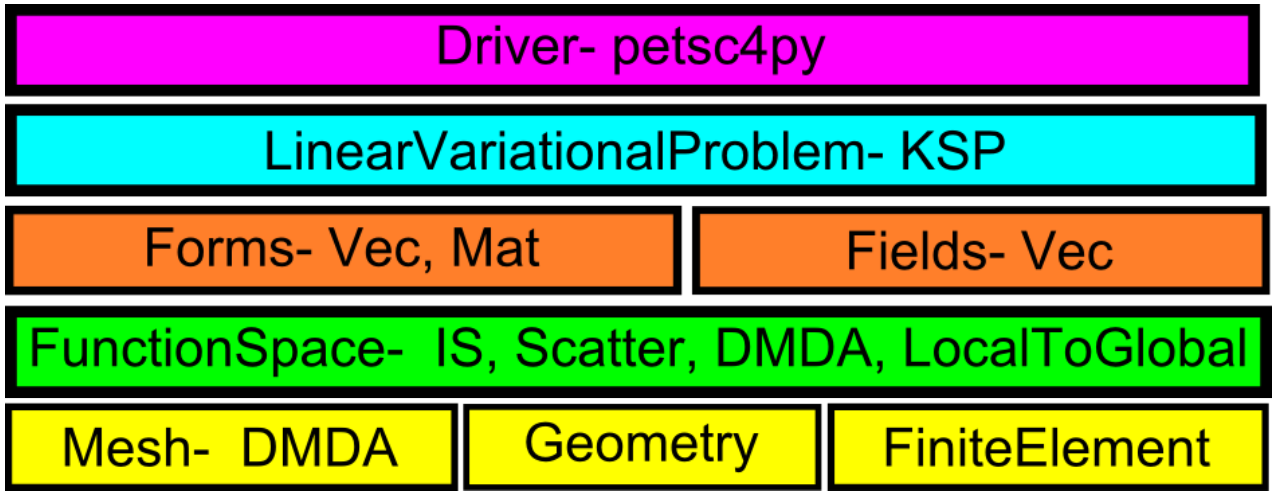
What is Themis?

1. PETSc-based software framework (written in Python and C)
2. Parallel, high-performance*, automated* discretization of variational forms
3. Using mimetic, tensor-product Galerkin methods on structured grids
4. Enables rapid prototyping and experimentation

Available online at `https://bitbucket.org/chris_eldred/themis`
- work in progress

Design Principles

1. Leverage existing software packages: PETSc, petsc4py, Numpy, Sympy, Instant, ...
2. Restrict to a subset of methods: mimetic, tensor-product Galerkin methods on structured grids
3. Similar in spirit and high-level design to FEniCS/Firedrake



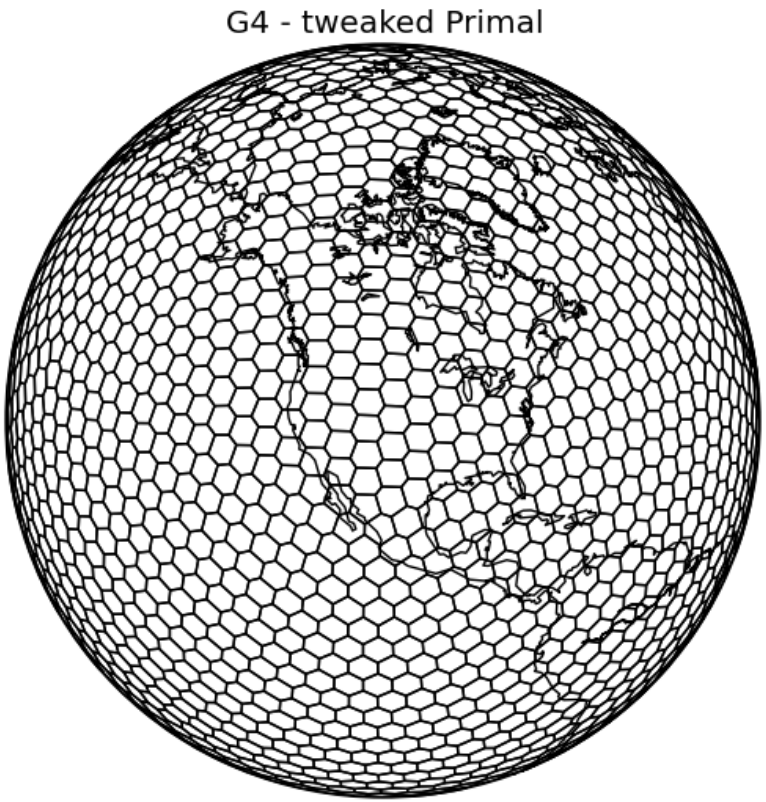
Current Capabilities

1. Support for structured grids in 1, 2 and 3 dimensions
2. Parallelism through MPI
3. Automated generation of assembly code (with user supplied kernels)
4. Arbitrary curvilinear mappings between physical and reference space
5. Support for mixed, vector and standard tensor-product Galerkin function spaces
6. Support for mimetic Galerkin difference elements, $Q_r^- \Lambda^k$ elements (both Lagrange and Bernstein basis) and mimetic spectral elements (single-grid version only)
7. Essential and periodic boundary conditions
8. Both tensor-product (sum-factorization)-based assembly and operator action

Planned Extensions

1. Facet integrals: enables natural boundary conditions
2. Multi-block domains: enables cubed-sphere
3. Nonlinear variational problems (via SNES): enables (semi)-implicit timestepping
4. Multiple element types (in the same domain): enables MGD elements with non-periodic boundaries
5. Additional work on optimization of data structures (Vecs/Mats/DMs) and assembly/operator action kernels (including vectorization and better shared memory support)
6. Bernstein polynomial based assembly and operator action
7. Weighted-row based assembly and operator action for MGD elements

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

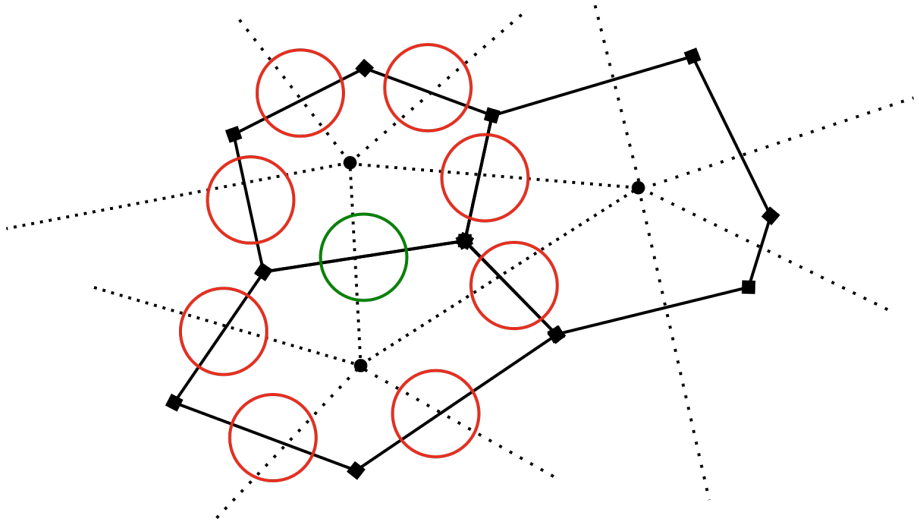
Reconstruction Operator ($\mathbf{W}$) in TRiSK

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

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

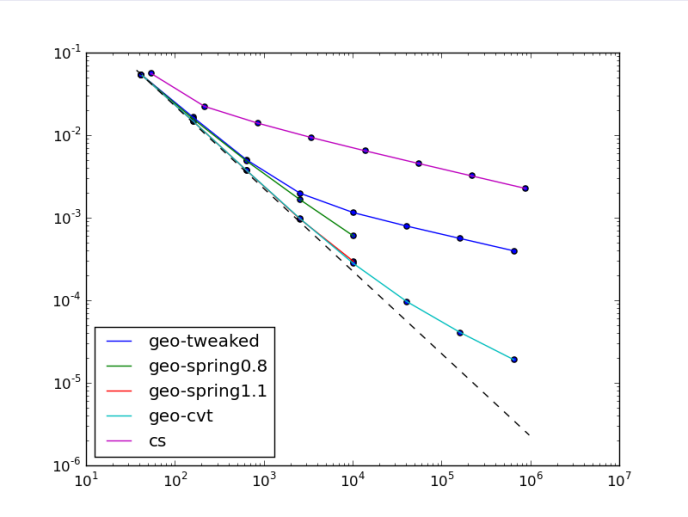
$$-\mathbf{R} D_2 = \bar{D}_2 \mathbf{W}$$

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

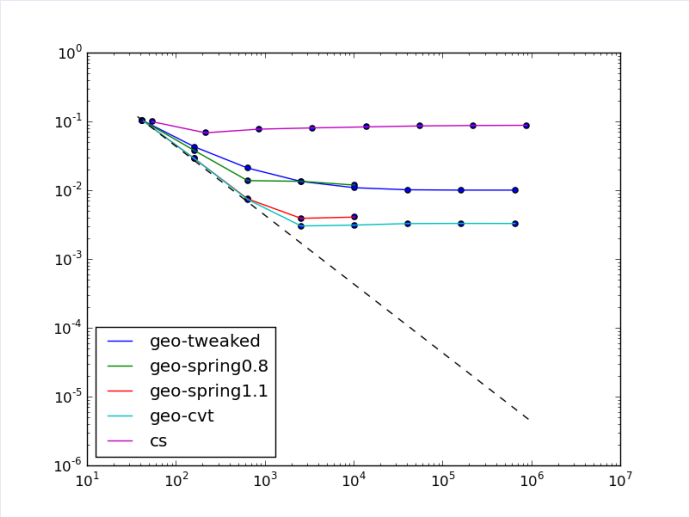


Issues with TRiSK

Operator Accuracy



L_2 for $\mathbf{W}$

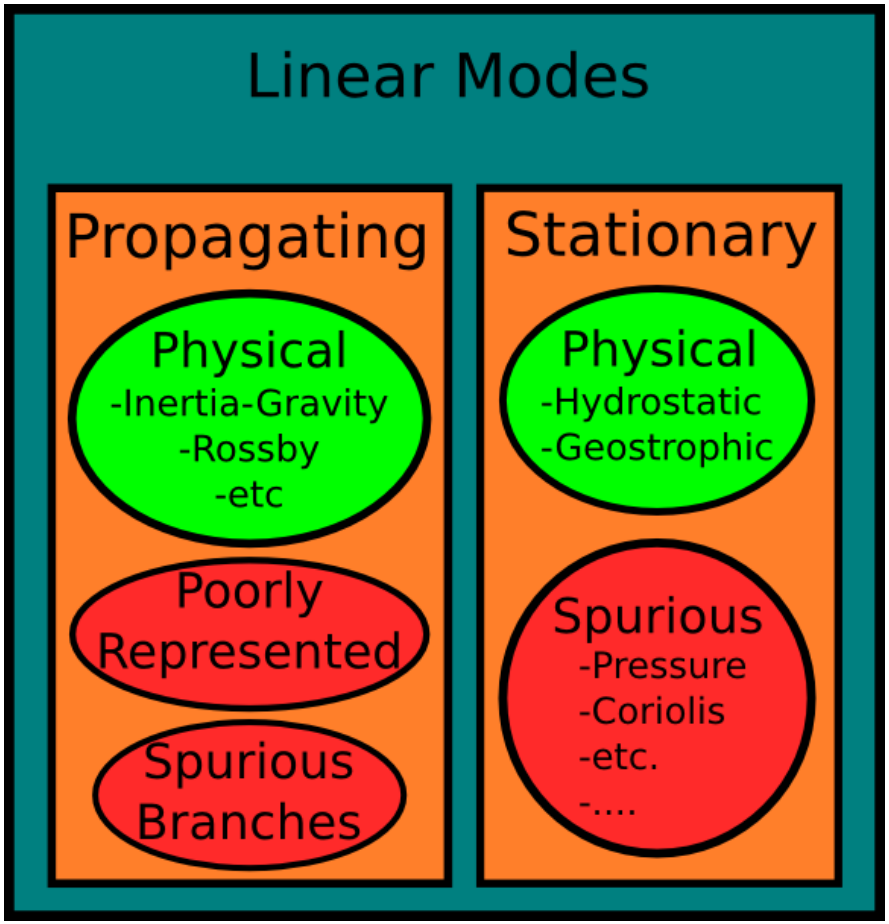


L_∞ for $\mathbf{W}$

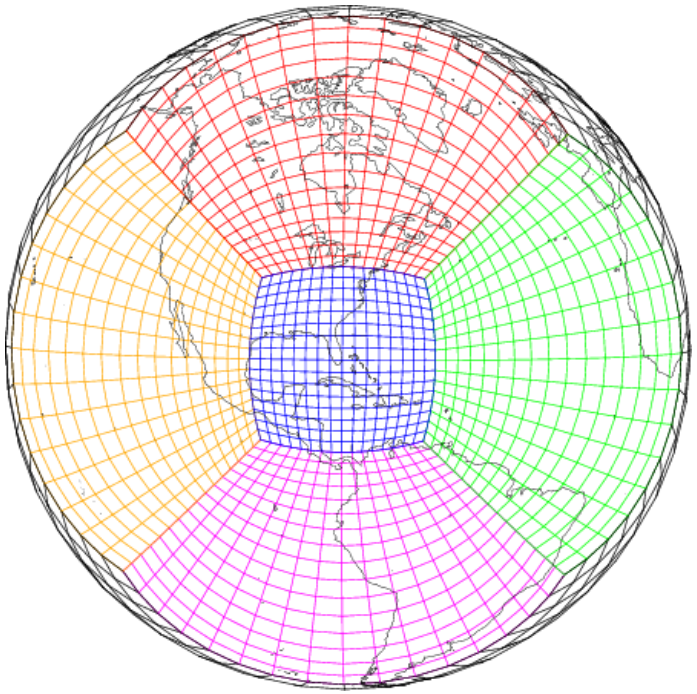
Spurious Branches of Dispersion Relationship

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

Linear Modes



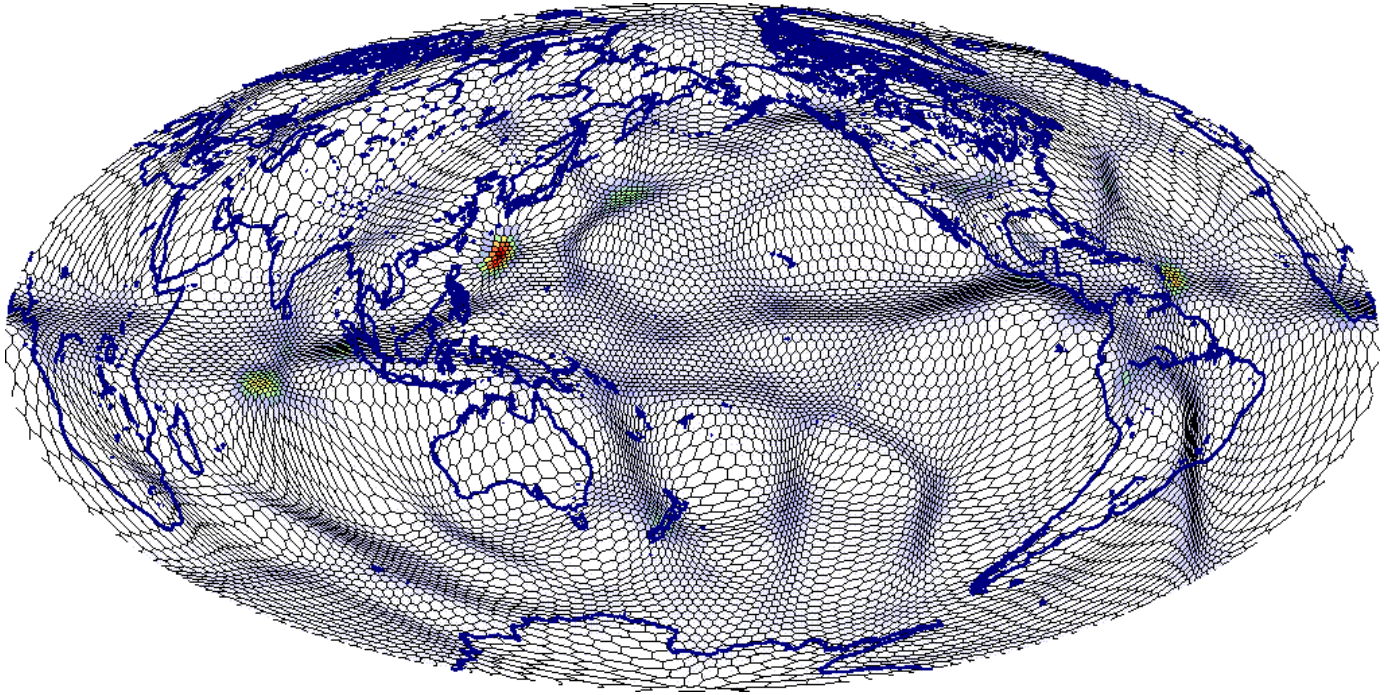
Static Refinement (r-refinement)



Stretched grids (picture from GDFL FV3, also known as Schmidt transform)

Grid topology is preserved $\rightarrow$ no change in computational efficiency

Adaptive Refinement (r-refinement)



Monge-Ampere mesh (picture from Weller)
Grid topology is preserved $\rightarrow$ no change in computational efficiency
Work by Cotter, McRae, Weller and other suggests that properties can be preserved even with adaptivity