Update on WP3.2: Themis and Hydrostatic Dynamical Core

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WP3.2 Milestones

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1. D3.3 (T0+6) Linear analysis and convergence of higher-order finite-element schemes, journal article
2. D3.4 (T0+12) Benchmarking of HO FE schemes for the RSW equations on the sphere, journal article
3. M3.2 (T0+24) Prototype, efficient 3D implementation of hydrostatic core using HO FE
4. D3.5 (T0+30) Cost and accuracy of HO-FE vs DYNAMICO in academic benchmark

WP3.2 Progress

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1. Software Framework: Themis
2. Mimetic Galerkin Differences: Analytic dispersion relationship (with Daniel Le Roux), efficiency work, theoretical properties
3. Dynamical Core: RSW done, working on Ripa and HPE
4. Papers in preparation: Mimetic Galerkin Differences: overall, RSW, linear modes; Themis

Software Framework

Themis

What is Themis?

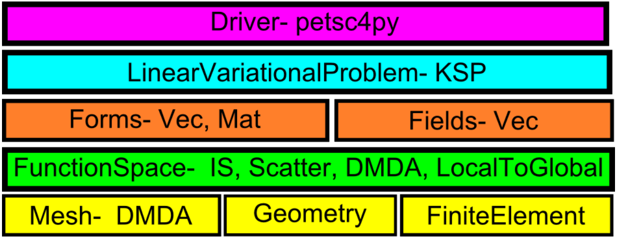
1. PETSc-based software framework (written in Python)
2. Parallel, high-performance*, automated* discretization of variational forms
3. Using mimetic, tensor-product Galerkin methods on structured grids
4. Enables rapid prototyping and experimentation

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. Support for essential and periodic boundary conditions

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. Duality/BLAS-based accelerated assembly and matrix-free variants: improved performance (CEMRACS project)
5. Multiple element types (in the same domain): enables MGD elements with non-periodic boundaries

Mimetic Galerkin Differences

Mimetic Galerkin Differences

Mimetic Galerkin Discretization

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

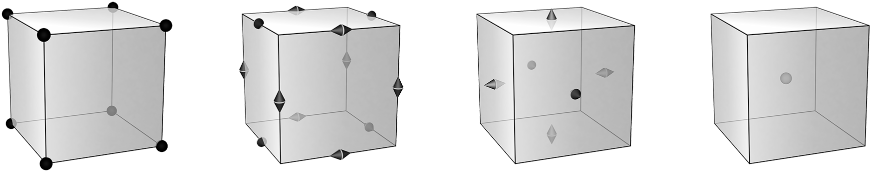
$$(da^k, b^{k+1}) = (a^k, \delta b^{k+1})$$

$$\delta = *d*$$

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

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

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



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

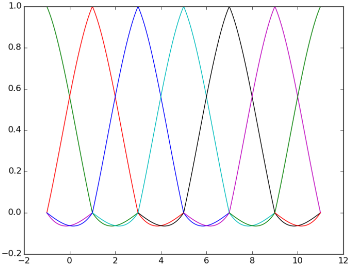
General Approach to Mimetic Galerkin Spaces

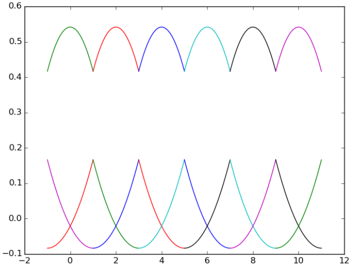
Mimetic Spaces

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

- 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)

Mimetic Galerkin Differences: Basis





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

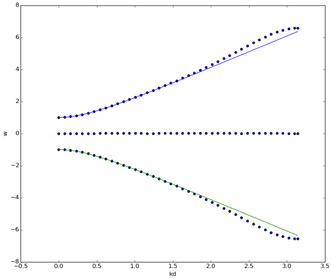
$\mathcal{B} = L_2$ Space (1D)

Single degree of freedom per geometric entity (physics coupling)

Higher order by larger stencils (less local)

3rd Order Elements

Mimetic Galerkin Differences- Dispersion



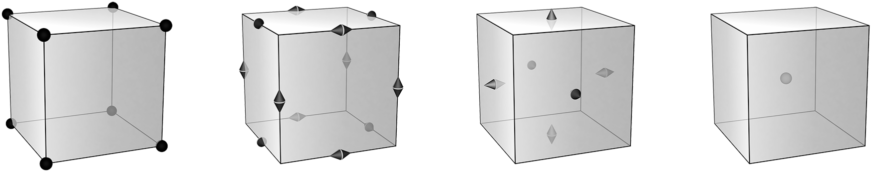
Inertia-Gravity Wave Dispersion Relationship (1D) for 3rd Order Elements

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



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

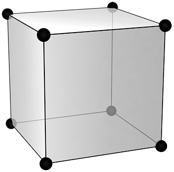
$$\mathbb{W}_0 \xrightarrow{\vec{\nabla}} \mathbb{W}_1 \xrightarrow{\vec{\nabla}\times} \mathbb{W}_2 \xrightarrow{\vec{\nabla}\cdot} \mathbb{W}_3$$

$\mathbb{W}_0 = \mathcal{A} \otimes \mathcal{A} \otimes \mathcal{A} = H_1 =$ Continuous Galerkin
$\mathbb{W}_1 = (\mathcal{B} \otimes \mathcal{A} \otimes \mathcal{A})\hat{i} + \ldots = H(curl) =$ 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

Dynamical Core

Dynamical Core

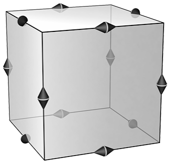
Grid Staggering for HPE



$\mathbb{W}_0$

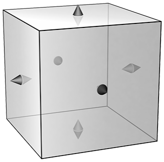
Θ

Differential Geometry



$\mathbb{W}_1$

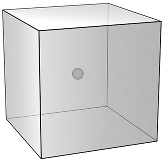
$\vec{\zeta}$



$\mathbb{W}_2$

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

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?

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

$$\frac{d\mathcal{F}}{dt} = \{\frac{\delta \mathcal{F}}{\delta \vec{x}}, \frac{\delta \mathcal{H}}{\delta \vec{x}}\}_{SW} + \{\frac{\delta \mathcal{F}}{\delta \vec{x}}, \frac{\delta \mathcal{H}}{\delta \vec{x}}\}_{\Theta} + \langle \frac{\delta \mathcal{F}}{\delta z} \frac{\partial z}{\partial t} \rangle \tag{2}$$

$$\{\frac{\delta \mathcal{F}}{\delta \vec{x}}, \frac{\delta \mathcal{H}}{\delta \vec{x}}\}_{SW} = \langle \frac{\delta \mathcal{H}}{\delta \vec{v}} \cdot \vec{\nabla} \frac{\delta \mathcal{F}}{\delta \mu} - \frac{\delta \mathcal{H}}{\delta \vec{v}} \cdot \vec{\nabla} \frac{\delta \mathcal{F}}{\delta \mu} \rangle + \langle \frac{\vec{\nabla} \times \vec{v}}{\mu} \cdot (\frac{\delta \mathcal{F}}{\delta \vec{v}} \times \frac{\delta \mathcal{H}}{\delta \vec{v}}) \rangle \tag{3}$$

$$\{\frac{\delta \mathcal{F}}{\delta \vec{x}}, \frac{\delta \mathcal{H}}{\delta \vec{x}}\}_{\Theta} = \langle \theta (\frac{\delta \mathcal{H}}{\delta \vec{v}} \cdot \vec{\nabla} \frac{\delta \mathcal{F}}{\delta \Theta} - \frac{\delta \mathcal{H}}{\delta \vec{v}} \cdot \vec{\nabla} \frac{\delta \mathcal{F}}{\delta \Theta}) \rangle \tag{4}$$

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:

$$\int \hat{\mu} \left(\frac{\partial \mu}{\partial t} + \vec{\nabla} \cdot \left(\frac{\delta \mathcal{H}}{\delta \vec{v}} \right) \right) = 0 \tag{5}$$

$$\int \hat{\Theta} \left(\frac{\partial \Theta}{\partial t} + \vec{\nabla} \cdot \left(\theta \frac{\delta \mathcal{H}}{\delta \vec{v}} \right) \right) = 0 \tag{6}$$

$$\int \hat{v} \left(\frac{\partial \vec{v}}{\partial t} + \frac{\zeta_v}{\mu} \times \frac{\delta \mathcal{H}}{\delta \vec{v}} + \theta \vec{\nabla} \left(\frac{\delta \mathcal{H}}{\delta \Theta} \right) + \vec{\nabla} \left(\frac{\delta \mathcal{H}}{\delta \mu} \right) \right) = 0 \tag{7}$$

$$\int \hat{z} \frac{\delta \mathcal{H}}{\delta z} = \int \hat{z} \left(g \mu + \frac{\partial p}{\partial \eta} \right) = 0 \tag{8}$$

Note that these are ALL 2D except for hydrostatic balance (8)

Hamiltonian (Lagrangian Vertical Coordinate)

Hamiltonian and Functional Derivatives

$$\mathcal{H} = \mathcal{H}[\mu, \vec{v}, \Theta, z] = \int \mu\Big(\frac{\vec{u}\cdot\vec{u}}{2} + U\Big(\frac{1}{\mu}\frac{\partial z}{\partial \eta}, \frac{\Theta}{\mu}\Big) + gz\Big) \tag{9}$$

$$\int \hat{v}\frac{\delta \mathcal{H}}{\delta \vec{v}} = \int \hat{v}\,(\mu\vec{u}) \tag{10}$$

$$\int \hat{\mu}\frac{\delta \mathcal{H}}{\delta \mu} = \int \hat{\mu}\left(\frac{\vec{u}\cdot\vec{u}}{2} + gz\right) \tag{11}$$

$$\int \hat{\Theta}\frac{\delta \mathcal{H}}{\delta \Theta} = \int \hat{\Theta}\frac{\partial U}{\partial \theta} = \int \hat{\Theta}\pi \tag{12}$$

$$\int \hat{z}\frac{\delta \mathcal{H}}{\delta z} = \int \hat{z}\left(g\mu + \frac{\partial p}{\partial \eta}\right) \tag{13}$$

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. Lorenz (Dynamico): $\mu, \Theta \in \mathbb{W}_3$ (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?)

Workplan

Workplan

Themis Workplan

CEMRACS: Summer 2016

1. Duality/BLAS-based assembly and matrix-free variant
2. Tensor-product assembly and matrix-free variant

Post-CEMRACS: Fall 2016

1. Multi-block domains: enables cubed-sphere
2. Multiple element types (in the same domain): enables MGD elements with non-periodic boundaries
3. Papers on Themis and on efficient assembly?

MGD Elements Workplan

Fall 2016

1. Finish theoretical properties: approximation rates (non-affine grids especially)
2. 2D dispersion analysis for RSW
3. Stationary modes for RSW
4. Meet again with Daniel Le Roux (September or October?)
5. Papers on MGD, MGD applied to RSW/Ripa and MGD Linear Modes?

Dynamical Core Workplan

Fall 2016

1. Ripa
2. Multilayer RSW and Ripa
3. HPE: Lagrangian and Mass-based vertical coordinates

Spring 2017

1. Explore Θ staggering and vertical FE linear modes
2. Explore stabilization: θ reconstruction, $\vec{Q}$ flux (APVM, SUPG), other stabilizations
3. Test cases: DCMIP, others?
4. Efficiency: additional work, comparisons with Dynamico
5. Papers on HPE FE Dycore and Vertical Linear Modes?