Progress towards a (Quasi-)Hydrostatic Dynamical Core using Structure-Preserving "Finite Elements"

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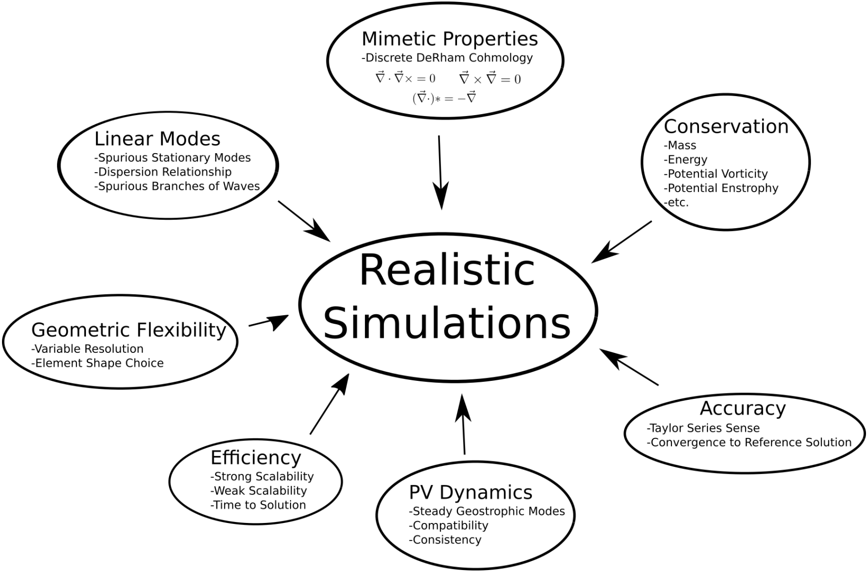
April 13th, 2017

Desirable Properties and Structure Preservation

Guiding Principles

1. Not solving arbitrary PDEs: building model of a physical system (no analytic solutions)
2. Differential equations → algebraic equations
3. **Do algebraic solutions have the same properties as the differential (true) solutions?**

(Incomplete) List of Desirable Model Properties



Obtaining these properties

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

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

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

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

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

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

Non-Canonical Hamiltonian Dynamics

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

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

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

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

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

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

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

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

$$
\begin{tikzcd}
\mathbb{W}_0 \arrow[r, "\vec{\nabla}", "d"'{yshift=3ex}] & \mathbb{W}_1 \arrow[r, "\vec{\nabla}\times", "d"'{yshift=3ex}] \arrow[l, dashed, bend left, "\vec{\nabla}\cdot", "\delta"'{yshift=-3ex}] & \mathbb{W}_2 \arrow[r, "\vec{\nabla}\cdot", "d"'{yshift=3ex}] \arrow[l, dashed, bend left, "\vec{\nabla}\times", "\delta"'{yshift=-3ex}] & \mathbb{W}_3 \arrow[l, dashed, bend left, "\vec{\nabla}", "\delta"'{yshift=-3ex}]
\end{tikzcd}
$$

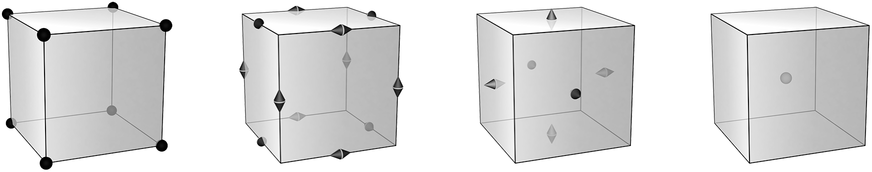
$$(da^k, b^{k+1}) = (a^k, \delta b^{k+1})$$

$$\delta = *d*$$

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

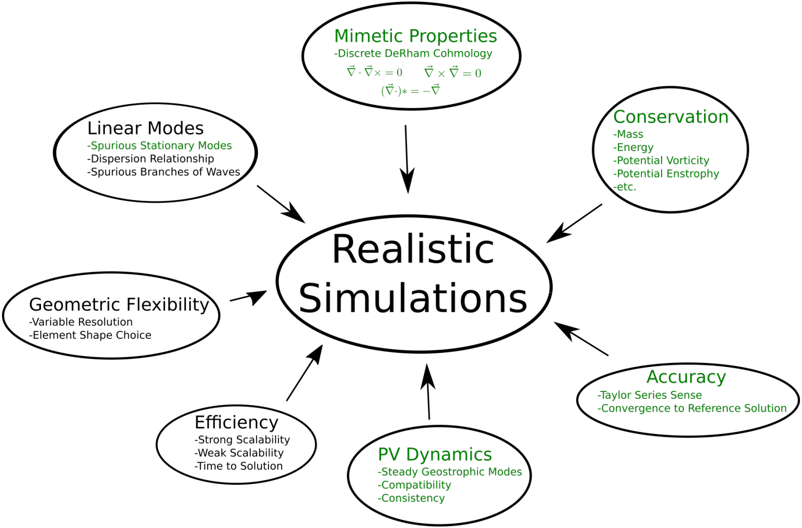
$$\vec{\nabla} \cdot \vec{\nabla}\times = 0 = \vec{\nabla} \times \vec{\nabla}$$

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



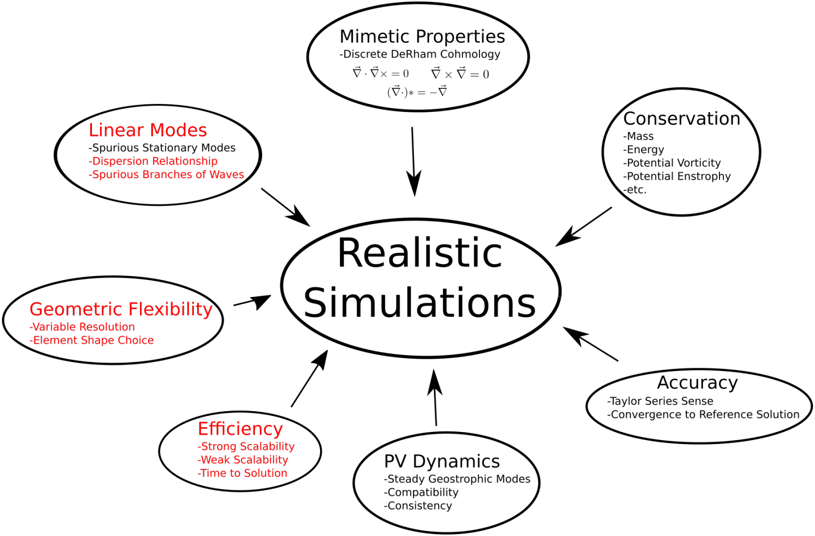
$\mathbb{W}_0$ $\mathbb{W}_1$ $\mathbb{W}_2$ $\mathbb{W}_3$

Hamiltonian + Mimetic : 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 Compatible Galerkin Methods

Tensor Product Compatible Galerkin Spaces

Tensor Product Compatible Galerkin Spaces

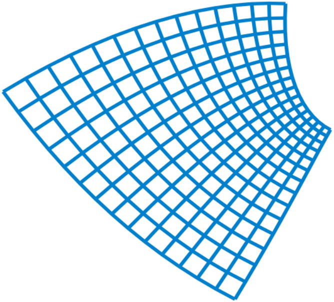
Given 1D Spaces $\mathcal{A}$ and $\mathcal{B}$ such that : $\mathcal{A} \xrightarrow{\frac{d}{dx}} \mathcal{B}$

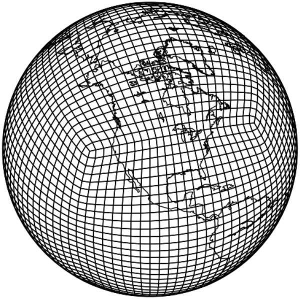
1. $\mathcal{A} = H^1$, $\mathcal{B} = L_2$
2. Use tensor products to extend to n-dimensions
3. Works for ANY set of spaces $\mathcal{A}$ and $\mathcal{B}$ that satisfy this property (compatible finite elements use P_n and $P_{DG,n-1}$; other choices yield mimetic spectral elements and compatible isogeometric methods)
4. Our (novel) choices of $\mathcal{A}$ and $\mathcal{B}$ are guided by linear mode properties and coupling to physics/tracer transport

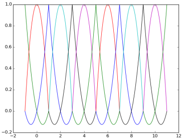
How do we get the remaining properties?

Tensor Product Compatible Galerkin Methods on Structured Grids

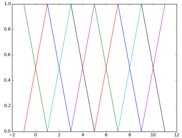
1. **Tensor product + structured grids**: efficiency
2. **Quadrilateral grids**- no spurious wave branches
3. **Key: What about dispersion relationships?**



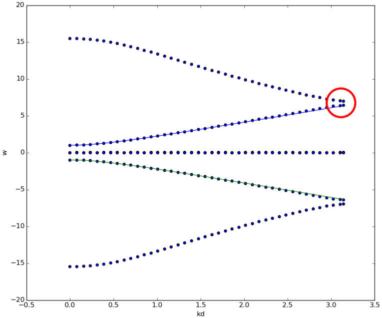




$\mathcal{A} = H_1$ Space (1D)



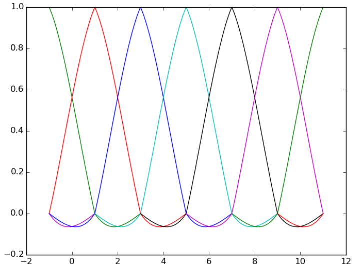
$\mathcal{B} = L_2$ Space (1D)



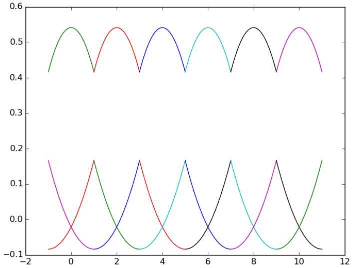
Inertia-Gravity Wave Dispersion Relationship (1D)

-Multiple dofs per element with different basis functions → breaks translational invariance → spectral gaps

-Can fix with mass lumping, but equation dependent and doesn't work for 3rd order and higher



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



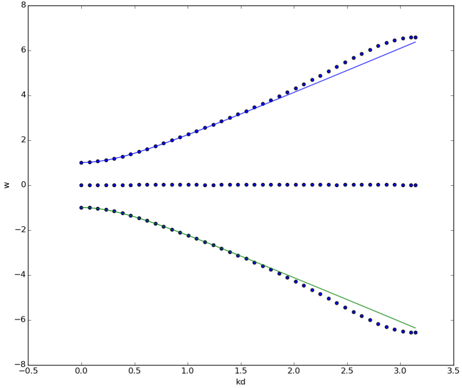
$\mathcal{B} = L_2$ Space (1D)

-Higher-order by increasing support of basis functions

-Single degree of freedom per geometric entity $\rightarrow$ dofs are identical to finite-difference (physics and tracer transport coupling)

-Higher order by larger stencils (less local, efficiency concerns)

Mimetic Galerkin Differences: Dispersion



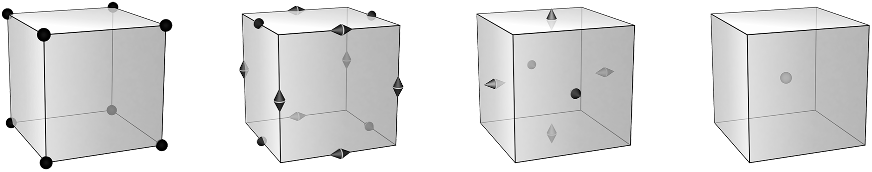
Inertia-Gravity Wave Dispersion Relationship (1D) for 3rd Order Elements

Spectral gap is gone

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

More details in a forthcoming paper with Daniel Le Roux

Overview of 3D Spaces



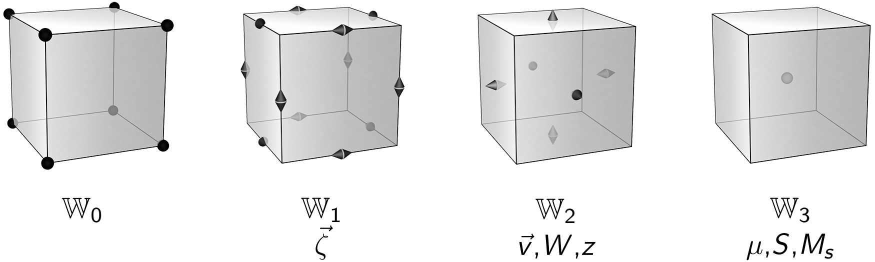
$\mathbb{W}_0$ $\mathbb{W}_1$ $\mathbb{W}_2$ $\mathbb{W}_3$

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

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

Actual Model and Results

Prognostic Variables and Grid Staggering



Prognose (1) μ or $M_s = \int_0^1 \mu d\eta$, (2) $\vec{v} = \vec{u} + \vec{R}$ and (3) $S = \mu s$ (or $\Theta = \mu\theta$)

Diagnose z from (quasi-)hydrostatic balance

Diagnose $W = \mu\dot{\eta}$ from vertical coordinate definition

Galerkin Version of a C/Lorenz Grid

Poisson Brackets

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

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

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

$$\{\frac{\delta \mathcal{F}}{\delta \vec{x}}, \frac{\delta \mathcal{H}}{\delta \vec{x}}\}s = \langle s(\frac{\delta \mathcal{H}}{\delta \vec{v}} \cdot \vec{\nabla} \frac{\delta \mathcal{F}}{\delta S} - \frac{\delta \mathcal{H}}{\delta \vec{v}} \cdot \vec{\nabla} \frac{\delta \mathcal{F}}{\delta S}) \rangle$$

where μ is the pseudo-density, $\vec{v} = \vec{u} - \vec{R}$ is the absolute (covariant) velocity, $S = \mu s$ is the mass-weighted entropy and z is the height. $W = 0$ defines the vertical coordinate.
-Get discrete equations by simply restricting brackets to finite-dimensional spaces, and letting $\mathcal{F} = \int \hat{\mu} \mu$, etc.

$$\left\langle \hat{\mu}, \frac{\partial \mu}{\partial t} \right\rangle + \left\langle \hat{\mu}, \vec{\nabla} \cdot (\frac{\delta \mathcal{H}}{\delta \vec{v}}) \right\rangle = 0$$

$$\left\langle \hat{S}, \frac{\partial S}{\partial t} \right\rangle + \left\langle \hat{S}, \vec{\nabla} \cdot (s \frac{\delta \mathcal{H}}{\delta \vec{v}}) \right\rangle = 0$$

$$\left\langle \hat{v}, \frac{\partial \vec{v}}{\partial t} \right\rangle - \left\langle \vec{\nabla} \cdot \hat{v}, \frac{\delta \mathcal{H}}{\delta \mu} \right\rangle + \left\langle \hat{v}, q\hat{k} \times (\frac{\delta \mathcal{H}}{\delta \vec{v}}) \right\rangle - \left\langle \vec{\nabla} \cdot (s\hat{v}), \frac{\delta \mathcal{H}}{\delta S} \right\rangle = 0$$

$$\mathcal{H} = \int \mu \left[\Phi(z) + K(\vec{v}, z) + U(\frac{1}{\mu}\frac{\partial z}{\partial \eta}, \frac{S}{\mu}) \right] + \int_{\Gamma^T} p_\infty z$$

-Blue terms are shallow water, Red terms are Ripa

-The μ equation holds pointwise, S and $\vec{v}$ require a linear solve

-Different choices of kinetic energy K and geopotential Φ give hydrostatic primitive (HPE), non-traditional shallow (NTE) and deep quasi-hydrostatic equations (QHE)

-$U(\alpha, s) = U(\frac{1}{\mu}\frac{\partial z}{\partial \eta}, \frac{S}{\mu})$ comes from the (arbitrary) equation of state

Equations of Motion: Lagrangian Vertical Coordinate (2)

Functional derivatives of $\mathcal{H}$ close the system and are given by:

$$\left\langle \hat{\mu}, \frac{\delta \mathcal{H}}{\delta \mu} \right\rangle = \langle \hat{\mu}, K + \Phi + U + p\alpha - sT \rangle$$

$$\left\langle \hat{S}, \frac{\delta \mathcal{H}}{\delta S} \right\rangle = \left\langle \hat{S}, T \right\rangle$$

$$\left\langle \hat{v}, \frac{\delta \mathcal{H}}{\delta \vec{v}} \right\rangle = \langle \hat{v}, \mu \vec{u} \rangle$$

$$\left\langle \hat{z}, \frac{\delta \mathcal{H}}{\delta z} \right\rangle = \left\langle \hat{z}, \mu \frac{\partial K}{\partial z} + \mu \frac{\partial \Phi}{\partial z} \right\rangle - \left\langle \frac{\partial \hat{z}}{\partial \eta}, p \right\rangle -$$
$$\langle \hat{z}, [[p]] \rangle_{\Gamma^I} - \langle \hat{z}, p \rangle_{\Gamma^B} + \langle \hat{z}, p_\infty \rangle_{\Gamma^T} = 0$$

-Some of these can be directly substituted into equations of motion, some require a linear solve

-Hydrostatic balance is $\frac{\delta \mathcal{H}}{\delta z} = 0$, requires a nonlinear solve

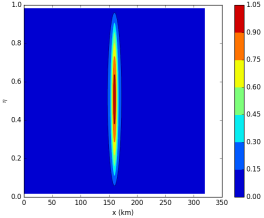
Conservation

Energy

- Arises purely from anti-symmetry of the brackets PLUS $\frac{\delta \mathcal{H}}{\delta z} = 0$
- Compatible 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

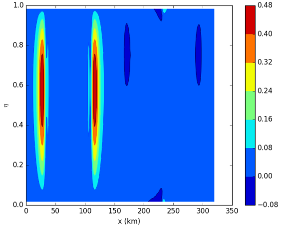
Mass and Entropy

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



$\theta'(t = 0)$

320km x 10km domain, 320x30 mesh ($\Delta x = 1$km), $\Delta t = 3s$, Lagrangian coordinate, MGD-1, results shown at 3600s, xz slice, 4th order Runge-Kutta



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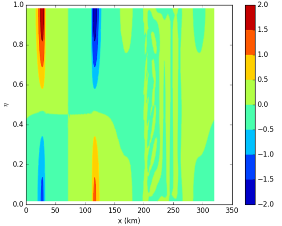


u'

Energy Conserving Time Stepping

Energy conserving spatial discretizations can be written as:

$$\frac{\partial \vec{x}}{\partial t} = \mathcal{J}(\vec{x}) \frac{\delta \mathcal{H}}{\delta \vec{x}}(\vec{x})$$

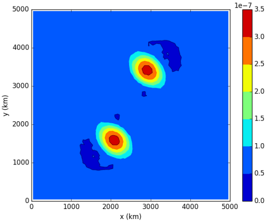
where $\mathcal{J} = \mathcal{J}^T$ and $\mathcal{H}$ is conserved. A 2nd-order, fully implicit energy conserving time integrator for this system is:

$$\frac{\vec{x}^{n+1} - \vec{x}^{n}}{\Delta t} = \mathcal{J}(\frac{\vec{x}^{n+1} + \vec{x}^{n}}{2}) \int \frac{\delta \mathcal{H}}{\delta \vec{x}} (\vec{x}^{n} + \tau(\vec{x}^{n+1} - \vec{x}^{n})) d\tau$$

Evaluate integral via a quadrature rule. Details are in Cohen, D. & Hairer, E. Bit Numer Math (2011)

-Hydrostatic balance and functional derivative solves can be incorporated into implicit solve → one single nonlinear solve

-Can simplify Jacobian to get a semi-implicit system without compromising energy conserving nature



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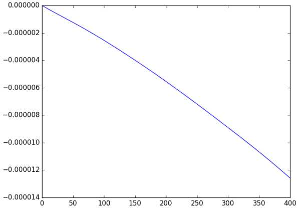
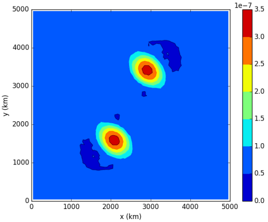
4th order Runge Kutta



$(E - E(0))/E(0) * 100.$



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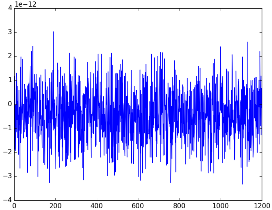
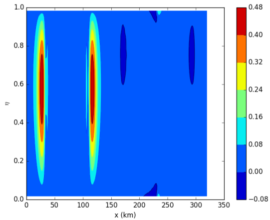
2nd order Energy Conserving (semi-implicit)



$(E - E(0))/E(0) * 100.$

Hydrostatic Gravity Wave Results



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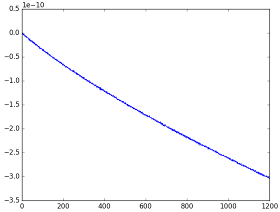
4th order
Runge Kutta



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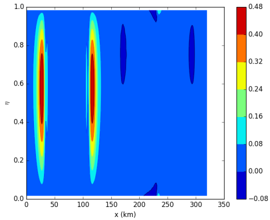

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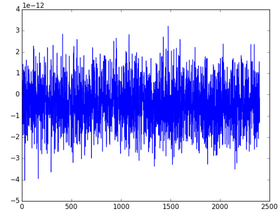
2nd order
Energy
Conserving



$(E - E(0))/E(0) * 100.$

Future Work, Summary and Conclusions

Dynamico-FE Review

1. Conservation of mass, entropy and energy
2. PV Dynamics: Steady geostrophic modes, compatible and consistent advection of PV
3. Linear Modes: Free of spurious stationary modes and branches of dispersion relations, excellent wave dispersion relationship
4. Has mimetic properties (such as $\vec{\nabla} \times \vec{\nabla} = 0$)
5. 2nd order accuracy in time, arbitrary accuracy in space (targeting 3rd order)
6. Lagrangian and Mass-based* vertical coordinate
7. Supports conforming block*-structured quadrilateral grids

**- work in progress*

Future Work

1. Mass-based vertical coordinate
2. Look at replacing S by s (Lorenz $\rightarrow$ Charney-Phillips)
3. Multipatch domains: cubed-sphere grid
4. Computational efficiency: simplified Jacobian, preconditioning, faster assembly and operator action
5. **Dispersion analysis for time/vertical/3D/4D discretization**
6. **Nonhydrostatic/soundproof equations**
7. **Past Reversible (Inviscid, Adiabatic) Dynamics: Subgrid Turbulence, Moisture/Tracers/Chemistry, 2nd Law of Thermodynamics, Physics-Dynamics Coupling (metriplectic, build on work by Francois Gay-Balmaz, Almut Gassmann, John Thuburn)**

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
4. Energy conserving time integration: possible, similar to existing semi-implicit schemes!

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

Motivating science question

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. Given (2), to what extent does (1) hold, especially since the real atmosphere has forcing and dissipation that makes it non-Hamiltonian (but possibly metricplectic)?
4. **Studying these questions requires a structure-preserving atmospheric model!**

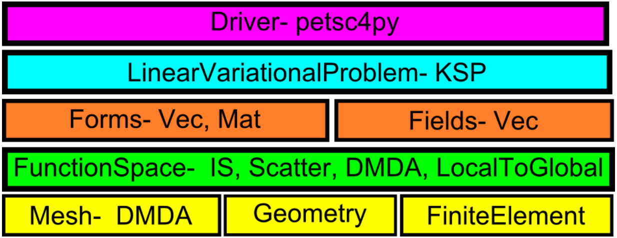
What is Themis?

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

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

**- work in progress*

1. Leverage existing software packages: PETSc, petsc4py, Numpy, Sympy, UFL, COFFEE, TSFC, 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 (in fact, shares UFL/COFFEE/TSFC)



Current Capabilities

1. Support for single block 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 and standard function spaces on those elements
5. Essential and periodic boundary conditions
6. Facet and volume integrals
7. Linear and nonlinear variational problems
8. Variational forms written in UFL and compiled using TSFC/COFFEE

Planned Extensions

1. Multiple element types (in the same domain): enables MGD elements with non-periodic boundaries
2. Matrix-free operator action
3. Multi-block domains: enables cubed-sphere
4. Geometric multigrid with partial coarsening
5. Weighted-row based assembly and operator action for MGD elements
6. Custom DM specialized for multipatch tensor product Galerkin methods
7. Further optimizations for assembly and operator action

Linear Modes