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

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Desirable Properties and Structure Preservation

Tensor Product Compatible Galerkin Methods

Actual Model and Results

Energy Conserving Time Stepping

Themis Software Framework

Future Work, Summary and Conclusions
Desirable Properties and Structure Preservation
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?
Realistic Simulations

Control Over Approximations
- Non-traditional/Deep
- Non-Spherical Geopotential
- Arbitrary Equations of State

Linear Modes
- No Spurious Stationary Modes
- Good Dispersion Relationship
- No Spurious Branches of Waves
- No Inertial Modes

Accuracy
- Taylor Series Sense
- Convergence to Reference Solutions

Conservation
- Mass
- Energy
- Potential Vorticity
- Entropy

Stability
- No Hollingsworth Instability
- Nonlinear Stability

PV Dynamics
- Steady Geostrophic Modes
- Compatibility
- Consistency

Mimetic Properties
- Discrete DeRham Cohomology
- Bounded Co-Chain Projections

\[ \vec{\nabla} \cdot \vec{\nabla} x = 0 \quad \vec{\nabla} \times \vec{\nabla} = 0 \]

\[ (\vec{\nabla} \cdot \star) = -\vec{\nabla} \]

Efficiency
- Strong Scalability
- Weak Scalability
- Time to Solution
What is structure-preservation?

Obtaining these properties

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

\[
\frac{d\mathcal{H}}{dt} = 0 \quad \frac{dC}{dt} = 0
\]

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

\[
\vec{\nabla} \times \vec{\nabla} = 0
\]

\[
\vec{\nabla} \cdot \vec{\nabla} \times = 0
\]

\[
(\vec{\nabla} \cdot)^* = -\vec{\nabla}
\]
The Beginning: Arakawa and Lamb 1981, Sadourney 1975

Mimetic Finite Differences: Ringler et. al 2010; Thuburn et. al 2012, 2014, many others


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

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

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

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

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

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

Neatly encapsulates conservation properties ($\mathcal{H}$ and $\mathcal{C}$).
General Formulation for Mimetic Discretizations: Primal deRham Complex (Finite Element Type Methods)

\[ \delta = \ast d \ast \]

\[ \nabla^2 = d\delta + \delta d \]

\[ \nabla \cdot \nabla \times = 0 = \nabla \times \nabla \]

\[ dd = 0 = \delta \delta \]

\[ (da^k, b^{k+1}) = (a^k, \delta b^{k+1}) \]
Hamiltonian + Mimetic: What properties do we get?

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There are MANY choices of spaces that give these properties: key point is the deRham complex
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**Mimetic Properties**
- Discrete DeRham Cohomology
- Bounded Co-Chain Projections

\[ \vec{\nabla} \cdot \vec{\nabla} \times \vec{v} = 0 \quad \vec{\nabla} \times \vec{\nabla} = 0 \]
\[ (\vec{\nabla} \cdot \vec{v})^* = -\vec{v} \]

**Stability**
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These are a function of the specific choice of spaces
Tensor Product Compatible Galerkin Methods
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?

C4 - 6x24x24 - thuburn Primal
Compatible FE: $P_2 - P_{1,DG}$ Dispersion Relationship

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

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

- Multiple dofs per element with different basis functions $\rightarrow$ breaks translational invariance $\rightarrow$ spectral gaps
- Can fix with mass lumping, but equation dependent and doesn’t work for 3rd order and higher
Mimetic Galerkin Differences

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

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

\[ W_0 = A \otimes A \otimes A = H_1 = \text{Continuous Galerkin} \]

\[ W_1 = (B \otimes A \otimes A)\hat{i} + \ldots = H(\text{curl}) = \text{Nedelec} \]

\[ W_2 = (A \otimes B \otimes B)\hat{i} + \ldots = H(\text{div}) = \text{Raviart-Thomas} \]

\[ W_3 = B \otimes B \otimes B = L_2 = \text{Discontinuous Galerkin} \]
Actual Model and Results
Prognostic Variables and Grid Staggering

Prognose (1) $\mu$ 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 $W = \mu \eta$ from vertical coordinate definition
Galerkin Version of a C/Lorenz Grid
Poisson Brackets: Lagrangian Vertical Coordinate

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

$$\frac{d\mathcal{F}}{dt} = \{\frac{\delta \mathcal{F}}{\delta \bar{x}}, \frac{\delta H}{\delta \bar{x}}\} \mathcal{W} + \{\frac{\delta \mathcal{F}}{\delta \bar{x}}, \frac{\delta H}{\delta \bar{x}}\} \mathcal{S} + \left< \frac{\delta \mathcal{F}}{\delta z} \frac{\partial z}{\partial t} \right>$$

$$\left< \frac{\delta \mathcal{F}}{\delta \bar{x}}, \frac{\delta H}{\delta \bar{x}} \right> \mathcal{W} = \left< \frac{\delta H}{\delta \bar{v}} \cdot \nabla \frac{\delta \mathcal{F}}{\delta \mu} - \frac{\delta H}{\delta \bar{v}} \cdot \nabla \frac{\delta \mathcal{F}}{\delta \mu} \right> + \left< \frac{\bar{v} \times \bar{v}}{\mu} \cdot \left( \frac{\delta \mathcal{F}}{\delta \bar{v}} \times \frac{\delta H}{\delta \bar{v}} \right) \right>$$

$$\left< \frac{\delta \mathcal{F}}{\delta \bar{x}}, \frac{\delta H}{\delta \bar{x}} \right> \mathcal{S} = \left< \mathcal{S} \left( \frac{\delta H}{\delta \bar{v}} \cdot \nabla \frac{\delta \mathcal{F}}{\delta S} - \frac{\delta H}{\delta \bar{v}} \cdot \nabla \frac{\delta \mathcal{F}}{\delta S} \right) \right>$$

where $\mu$ is the pseudo-density, $\bar{v} = \bar{u} - \bar{R}$ 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.
Equations of Motion: Lagrangian Vertical Coordinate (1)

\[
\langle \hat{\mu}, \frac{\partial \mu}{\partial t} \rangle + \langle \hat{\mu}, \vec{\nabla} \cdot (\frac{\delta H}{\delta \vec{v}}) \rangle = 0
\]

\[
\langle \hat{S}, \frac{\partial S}{\partial t} \rangle + \langle \hat{S}, \vec{\nabla} \cdot (s \frac{\delta H}{\delta \vec{v}}) \rangle = 0
\]

\[
\langle \hat{v}, \frac{\partial \vec{v}}{\partial t} \rangle - \langle \vec{\nabla} \cdot \hat{v}, \frac{\delta H}{\delta \mu} \rangle + \langle \hat{v}, qk \times (\frac{\delta H}{\delta \vec{v}}) \rangle - \langle \vec{\nabla} \cdot (s \hat{v}), \frac{\delta H}{\delta S} \rangle = 0
\]

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

- Blue terms are shallow water, Red terms are Ripa
- The \( \mu \) equation holds pointwise, \( S \) and \( \vec{v} \) require a linear solve
- Different choices of kinetic energy \( K \) and geopotential \( \Phi \) give hydrostatic primitive (HPE), non-traditional shallow (NTE) and deep quasi-hydrostatic equations (QHE)
- \( U(\alpha, s) = U\left(\frac{1}{\mu} \frac{\partial z}{\partial \eta}, \frac{S}{\mu}\right) \) comes from the (arbitrary) equation of state
Functional derivatives of $\mathcal{H}$ close the system and are given by:

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

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

$$\left\langle \nu, \frac{\delta \mathcal{H}}{\delta \nu} \right\rangle = \left\langle \nu, \mu \nu \right\rangle$$

$$\left\langle \hat{Z}, \frac{\delta \mathcal{H}}{\delta Z} \right\rangle = \left\langle \hat{Z}, \mu \frac{\partial K}{\partial Z} + \mu \frac{\partial \Phi}{\partial Z} \right\rangle - \left\langle \frac{\partial \hat{Z}}{\partial \eta}, p \right\rangle - \left\langle \hat{Z}, [[[p]]] \right\rangle_{\Gamma_I} - \left\langle \hat{Z}, p \right\rangle_{\Gamma_B} + \left\langle \hat{Z}, p_\infty \right\rangle_{\Gamma_T} = 0$$

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
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
Hydrostatic Gravity Wave

\[ \theta'(t = 0) \]

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

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

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
Shallow Water Results

4th order Runge Kutta

\[
q
\]

2nd order Energy Conserving (semi-implicit)

\[
(\frac{E - E(0)}{E(0)} \times 100.
\]

\[
(\frac{E - E(0)}{E(0)} \times 100.
\]
Hydrostatic Gravity Wave Results

4th order Runge Kutta

\[ (E - E(0))/E(0) \times 100. \]

2nd order Energy Conserving

\[ (E - E(0))/E(0) \times 100. \]
Themis Software Framework
What is Themis?

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

Themis is online at https://bitbucket.org/chris_eldred/themis
Firedrake is at http://www.firedrakeproject.org/
Design Principles

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 block-structured grids

3. Similar in spirit and high-level design to FEniCS/Firedrake (shares UFL/COFFEE/TSFC)

4. Access to symbolic representation of forms: automatic adjoints and derivatives, seamless switching between assembled and matrix-free, clever physics-based preconditioners, many other advantages

5. Intended to offer "good enough" performance for many science applications (prototyping atmospheric dynamical cores is initial target application)
Software Overview

(Non)linear variational problems in UFL plus problem solving language (similar to FEniCS/Firedrake)

Themis Software Stack

Form, Arguments, Coefficients, FiniteElement

Mesh, FunctionSpace, Field, EssentialBC

TSFC

Loop Nests

Optimized Local Assembly Kernels

Themis (PETSc/petsc4py)

Mat, Vec, DMDA, DMComposite

KSP, SNES

Global Assembly and Solution

Parallel, high-performance, automated discretization of variational forms using tensor-product compatible Galerkin methods on structured grids
Example Code: $H^1$ Helmholtz (in Firedrake, Themis and FEniCS very similar)

```python
mesh = UnitSquareMesh(10, 10)
V = FunctionSpace(mesh, "CG", 1)

u = TrialFunction(V)
v = TestFunction(V)

x, y = SpatialCoordinate(mesh)
f = (1+8*pi*pi)*cos(x*pi*2)*cos(y*pi*2)

a = (dot(grad(v), grad(u)) + v * u) * dx
L = f * v * dx

u = Function(V)
solve(a == L, u)
```
Current Capabilities

1. Support for multiblock* 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. Matrix-free operator action instead of assembly*
8. Linear and nonlinear variational problems

*- work in progress for UFL-based version
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. Semi-implicit version of energy-conserving time stepping
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. Hollingsworth Instability
6. Dispersion analysis for time/vertical/3D/4D discretization
7. Nonhydrostatic equations
8. Irreversible Dynamics and Physics-Dynamics Coupling: Metriplectic formulation (collaborating with Francois Gay-Balmaz, builds on work by Almut Gassmann)
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
General Formulation for Mimetic Discretizations: Primal-Dual Double deRham Complex (Staggered Grids)

\[ \delta = *d* \]
\[ \nabla^2 = d\delta + \delta d \]
\[ \nabla \cdot \nabla \times = 0 = \nabla \times \nabla \]

Outer Oriented Fluxes

Inner Oriented Circulations

\[ \int_{\Omega} dW = \int_{d\Omega} W \]
\[ dd = 0 = \delta\delta \]
Issues with TRiSK

Operator Accuracy

$L_2$ for $W$

$L_\infty$ for $W$

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
For canonical, finite-dimensional Hamiltonian systems, structure-preserving numerics are essential to obtain correct long-term statistical behavior.

The equations of (moist) adiabatic, inviscid atmospheric dynamics are a non-canonical, infinite-dimensional Hamiltonian system.

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)?

Studying these questions requires a structure-preserving atmospheric model!
Linear Modes

Structure Preserving Dynamical Cores

Linear Modes

Propagating
- Physical
  - Inertia-Gravity
  - Rossby
  - etc

- Poorly Represented

- Spurious Branches

Stationary
- Physical
  - Hydrostatic
  - Geostrophic

- Spurious
  - Pressure
  - Coriolis
  - etc.
  - etc.