Higher-order Finite Elements for Atmopsheric Dynamical Cores

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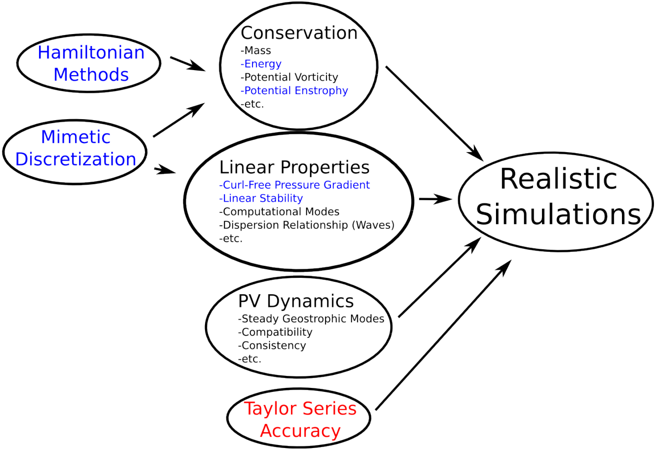
My Background

Background

- B.S. : Computational Physics, Carnegie Mellon University
- PhD : Atmospheric Science, Colorado State University
- I worked with David Randall on (quasi-)Hamiltonian discretizations for the rotating shallow water equations
- C and Z grid total energy and potential enstrophy schemes (extension of 1981 Arakawa and Lamb to arbitrary grids)
- Linear modes for these schemes on cubed-sphere and icosahedral grids (both stationary and propagating)
- Joined HEAT project in October 2015

Elements of Dynamical Core Design



Underlying 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, finite-dimensional Hamilontian system
3. To what extent does (1) hold for model of the atmosphere, given (2)?
4. Weather vs. climate simulations, planetary atmospheres, forced-dissipative systems, role of various approximations, what properties should we conserve and why?
5. **Studying these questions requires a structure-preserving atmospheric model!**

Mixed Finite Elements

De Rham Cohomology

$$\text{Strong} : \mathbb{V}_0 \xrightarrow{\vec{\nabla}^T} \mathbb{V}_1 \xrightarrow{\vec{\nabla}\cdot} \mathbb{V}_2$$

$$\text{Weak} : \mathbb{V}_0 \xleftarrow{\vec{\nabla}^T\cdot} \mathbb{V}_1 \xleftarrow{\vec{\nabla}} \mathbb{V}_2$$

C Grid Analogue

- $\mathbb{V}_0 = \psi/\zeta = H_1 =$ continuous (Lagrange)
- $\mathbb{V}_1 = \vec{u} = H(div) =$ continuous normals, discontinuous tangents (Raviart-Thomas)
- $\mathbb{V}_2 = h/\delta/\chi = L_2 =$ discontinuous (Discontinuous Lagrange)
- Could invert the diagram (define $\mathbb{V}_0 \xrightarrow{\vec{\nabla}} \mathbb{V}_1 \xrightarrow{\vec{\nabla}^T\cdot} \mathbb{V}_2$ strong, gives $H(curl)$/Nedelec spaces and D grid analogue)

FV-FE Spaces

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

Tensor Product 2D Spaces

- $\mathbb{V}_0 = \mathcal{A} \otimes \mathcal{A}$
- $\mathbb{V}_1 = \mathcal{A}\hat{i} + \mathcal{B}\hat{j}$ and $\mathcal{B}\hat{i} + \mathcal{A}\hat{j}$
- $\mathbb{V}_2 = \mathcal{B} \otimes \mathcal{B}$
- This works generally for ANY set of spaces $\mathcal{A}$ and $\mathcal{B}$ (usually P_n and $P_{DG,n-1}$)
- Our (different) choices of $\mathcal{A}$ and $\mathcal{B}$ guided by linear mode properties and coupling to physics/tracer transport

WP3 Milestones and Progress

WP3 Milestones

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

WP3 Progress (from Evaggelos)

1. Nothing new from January
2. 1D dispersion relationship
3. Basic convergence testing on cubed-sphere
4. Basic test cases (Galewsky, Williamson) on cubed-sphere
5. Possible meeting with Daniel Le Roux to discuss dispersion relationship?

My Workplan

Workplan Stage 1: 2D Shallow Water

1. Theory of 2D FV-FE spaces and scheme
   - Do the FV-FE spaces form a De Rham complex? What about steady geostrophic modes and PV compatibility? Proof of various properties
   - What are the linear modes? Analytic for 1D and 2D f-plane, numerical for cubed-sphere variable and constant f, proof of various properties
2. (Parallel) 2D Shallow Water Model
   - Re-implement current Matlab code in parallel
   - Explore preconditioning and solver options
   - Detailed testing and comparison with existing schemes, especially GungHo work
   - Start looking at stabilization/dissiptation

My Workplan

Workplan Stage 2: 3D Hydrostatic Primitive

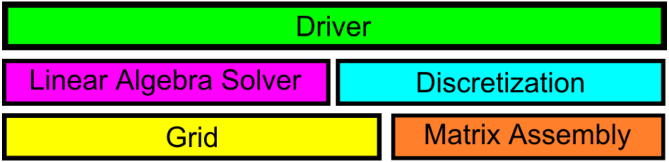
1. 2D Vertical Slice Model
    - Theory of how finite element spaces should look, what variables go where
    - Implementation using tensor-product grid and spaces approach
    - Explore advection choices for thermodynamic variables (entropy, moisture, etc.)
2. 3D Hydrostatic Primitive Equations Model
    - Combine 2D SW and 2D Vertical Slice
    - Multilayer uncoupled SW $\rightarrow$ Multilayer coupled SW $\rightarrow$ Lagrangian HPE $\rightarrow$ Hybrid mass-based HPE
    - Start looking at stabilization/dissiptation
    - Efficiency- explore solvers and preconditioners

Implementation Details

Implementation Plan- 2D Shallow Water

Design Goals

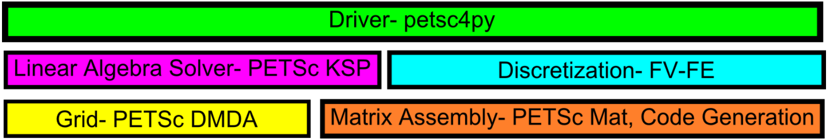
1. Flexibility in choice of grid, equations to be solved and discretization used (enables intercomparison)
2. Flexibility in choice of linear algebraic solvers
3. Leverage existing software packages
4. Focus on ease of development and proving feasibility, not pure performance
5. Inspired by Firedrake/FEniCS/GungHo (UK Met Office) approach



Implementation Plan- 2D Shallow Water

Preliminary Approach

1. Portable Extensible Toolkit for Scientific Computation: PETSc
2. Use PETSc (through petsc4py) along with code generation
3. Separate parts can be independently changed: new discretizations by altering grid/matrix assembly, new solvers, new equations by changing matrix assembly and driver, etc.

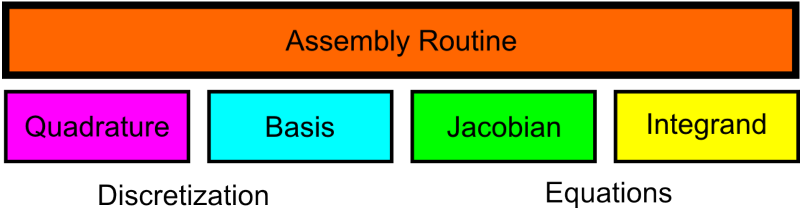


General Parallel Assembly Code (Vectors or Matrices)

```
Ul <- Ug
for element_type in element_types
    for element in subdomain(element_type)
        Ue <- Ul
        Ge = geometry(element)
        Fe = 0
        for xq,wq in quadrature(element)
            Jq = jacobian(element,xq)
            bq,bdq = basis(element,xq)
            iq = integrand(bq,bdq,xq)
            Fe += wq*Jq*iq
        Fe -> Fl
Fl -> Fg
```

Implementation Plan- 2D Shallow Water

- Change basis/quadrature: new discretization
- Change integrand/jacobian: new equations
- Lots of opportunity for optimization: vectorize calculations over quadrature points, inline constant parts, etc.
- Use code generation for given choice of basis, quadrature, Jacobian and integrand $\rightarrow$ efficient but extremely flexible



Implementation Plan- 2D Vertical Slice

2D Vertical Slice Model

1. Combine Cotter and Shipton approach (spaces) with Dubos (Hamiltonian) equation formulation and prognostic variables
2. FE both in horizontal and vertical

Given

$$1\text{D} : \mathcal{A} \xrightarrow{\frac{d}{dx}} \mathcal{B} \quad \text{and} \quad 2\text{D} : \mathbb{V}_0 \xrightarrow{\vec{\nabla}^T} \mathbb{V}_1 \xrightarrow{\vec{\nabla}\cdot} \mathbb{V}_2$$

Produce

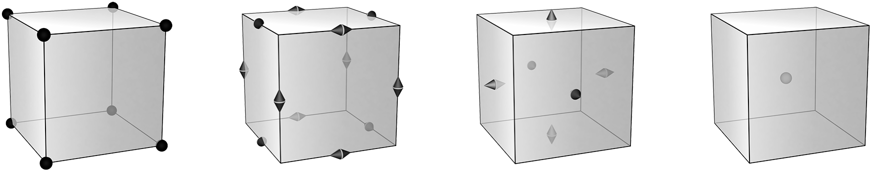
$$3\text{D} : \mathbb{W}_0 \xrightarrow{\vec{\nabla}} \mathbb{W}_1 \xrightarrow{\vec{\nabla}\times} \mathbb{W}_2 \xrightarrow{\vec{\nabla}\cdot} \mathbb{W}_3$$

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

Implementation Plan- 3D Hydrostatic

3D Model

1. Combine 2D shallow water and 2D vertical slice
2. Use extruded mesh idea from Firedrake (structured vertical columns)
3. Lorenz Grid = S in $\mathbb{W}_3$ (S could also be placed in vertical part of $\mathbb{W}_2$ = Charney-Phillips grid)



$\mathbb{W}_0$	$\mathbb{W}_1$	$\mathbb{W}_2$	$\mathbb{W}_3$
ψ	$\vec{\zeta}$	u_i, W	μ, S, δ, χ

Future Work

Possible extensions

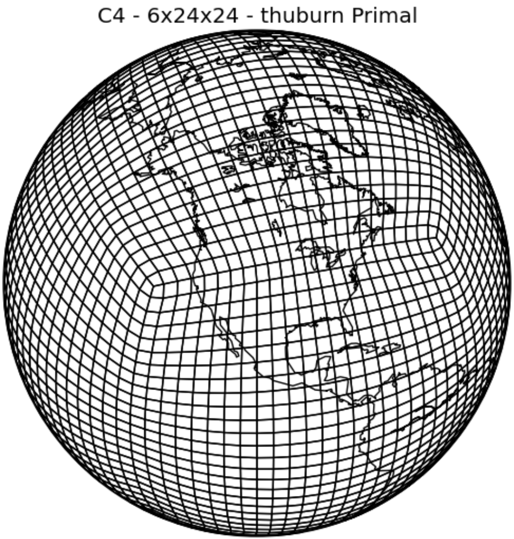
- New equation sets and approximations- non-spherical geoid, deep atmosphere, non-traditional Coriolis, non-hydrostatic
- Different discretizations: FEEC, compound FE, polygonal FE (many varieties here), IGA, mimetic SE, TRiSK, mimetic FV/DEC, etc.
- Time stepping- semi-implicit, symplectic, fully conservative
- FAS multigrid (to solve semi-implicit)
- 2D FV-FE spaces
- Multicomponent flows- moisture

Appendix

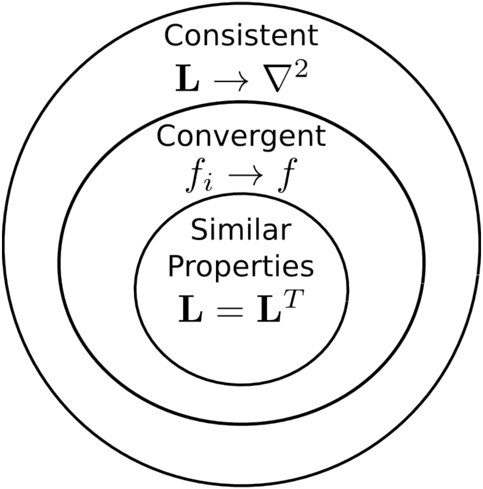
Grid Types

TYPE 1: logically square, extended stencil, each function space has degrees of freedom associated with a single type of geometric entity (this supports IGA, compatible SE and FV-FE; also certain compatible FE, compound FE and TRiSK spaces)- DMDA
Restriction to single type of geometric entity is mostly a software restriction due to issues with DMDA and support for staggered geometric stuff in DMDA
TYPE 2: unstructured polygonal, covering relation, each function space has degrees of freedom associated with many types of geometric entities (this supports compatible FE, TRiSK, compound FE)- DMPLEX ie cubed-sphere, geodesic and diamond

Grid



Numerical Methods

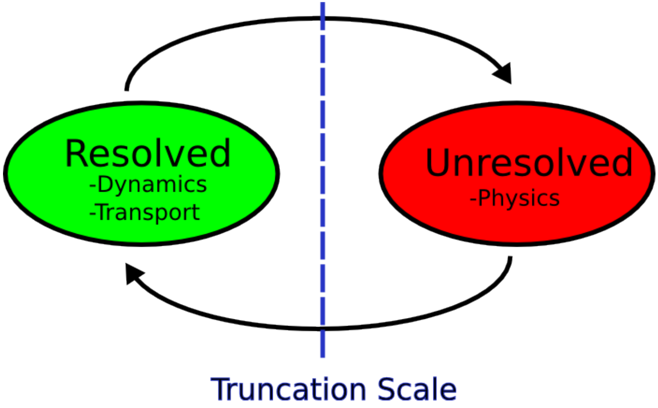


$$\Delta x, \Delta t \to 0$$

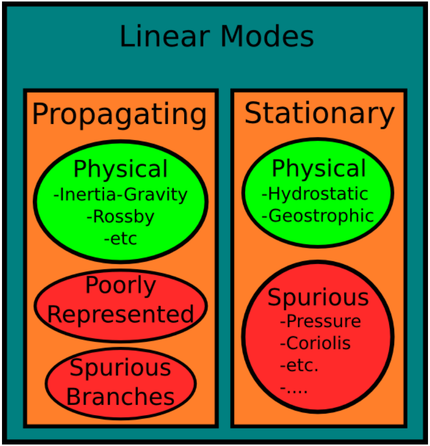
Primal Dual FE

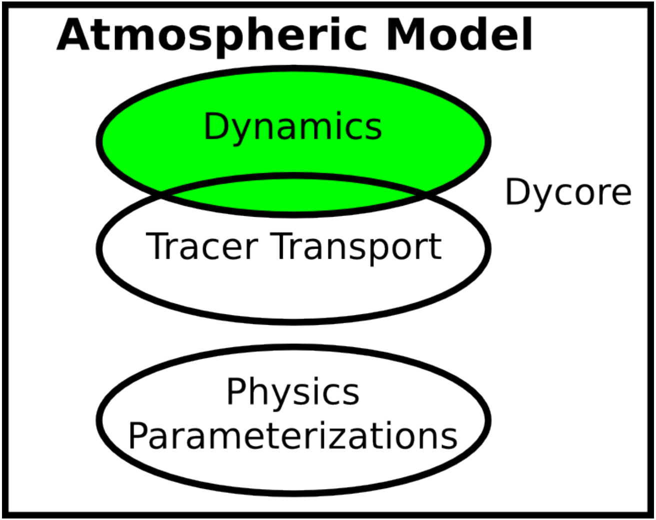
$$\begin{tikzcd}
\mathbf{V}^2 \arrow[r, dashed, bend left, "\nabla^{\perp}"] \arrow[d] & \mathbf{V}^1 \arrow[l, "\mathbf{k}\cdot\nabla\times"] \arrow[r, dashed, bend left, "\nabla\cdot"] \arrow[d] & \mathbf{V}^0 \arrow[l, "\nabla"] \arrow[d] \\
\mathbf{V}_0 \arrow[r, "\nabla^{\perp}"] & \mathbf{V}_1 \arrow[r, "\nabla\cdot"] \arrow[l, dashed, bend left, "\mathbf{k}\cdot\nabla\times"] & \mathbf{V}_2 \arrow[l, dashed, bend left, "\nabla"]
\end{tikzcd}$$

Resolved/Unresolved



Linear Modes




Atmospheric Model
Dynamics
Dycore
Tracer Transport
Physics
Parameterizations