Finite Element Hydrostatic Primitive Equations in Themis

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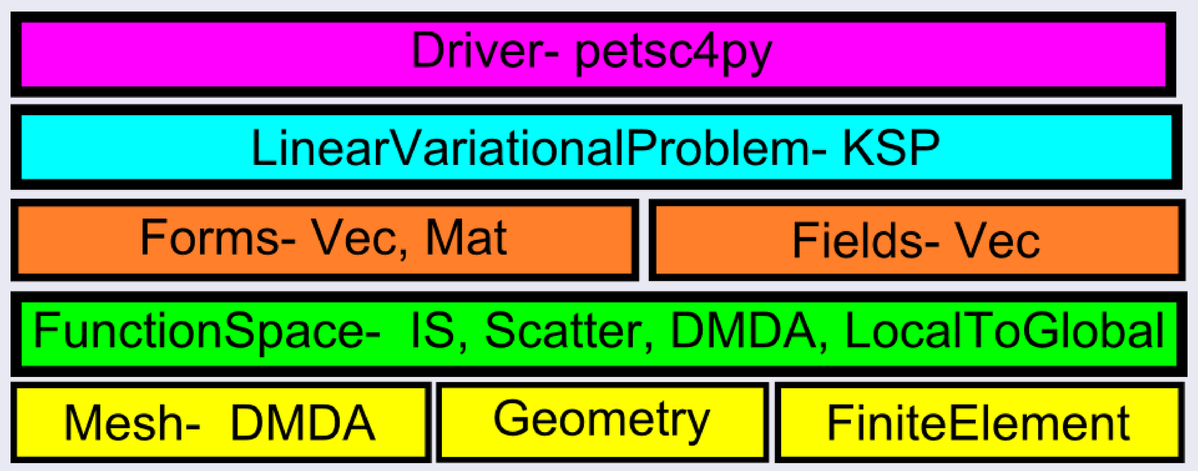
Themis: Accelerated Computational Science

Themis is a PETSc-based software framework (written primarily in Python using petsc4py) for parallel, high-performance*, automated* discretization of variational forms (and solution of systems of equations involving them) through mimetic, tensor-product Galerkin methods. It is intended to enable a rapid cycle of prototyping and experimentation, accelerating both the development of new numerical methods and scientific models that incorporate them.

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

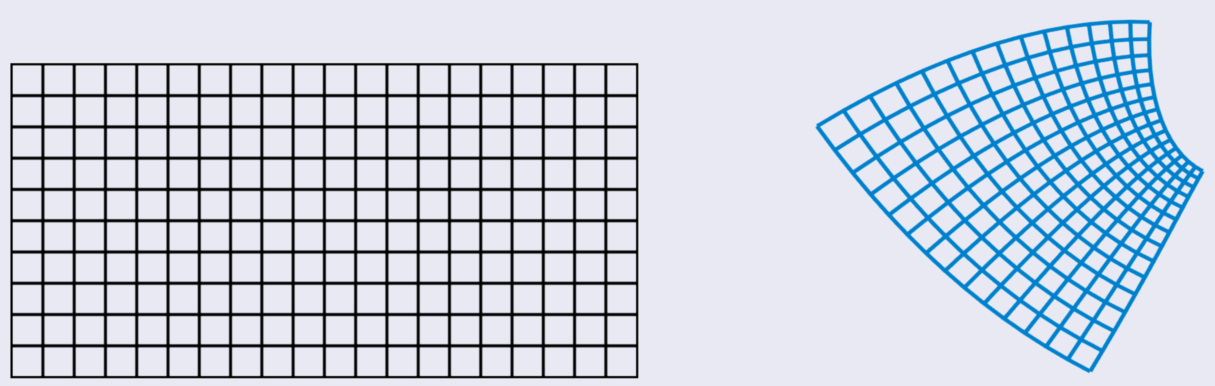
Design Principles behind Themis

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 of Themis

1. Support for single-block, structured grids in 1, 2 and 3 dimensions
2. Parallelism through MPI
3. Automated generation of assembly code (with user supplied kernels)
4. Arbitrary mappings between physical and reference space
5. Support for mixed, vector and standard tensor-product Galerkin function spaces using mimetic Galerkin difference elements (see [2] and [3]) and arbitrary order $Q_r^- \Lambda^k$ elements
6. Support for essential and periodic boundary conditions

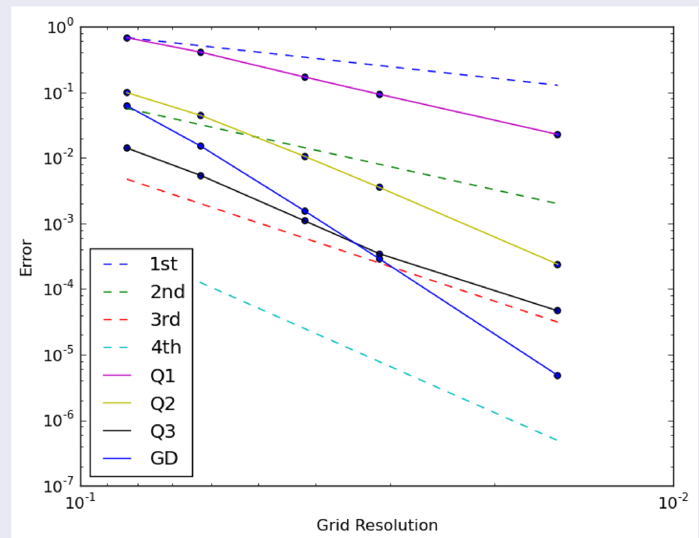


Some Results using Themis

H^1 Helmholtz Problem

$$< \vec{\nabla} \hat{h}, \vec{\nabla} h > = < \hat{h}, f >$$

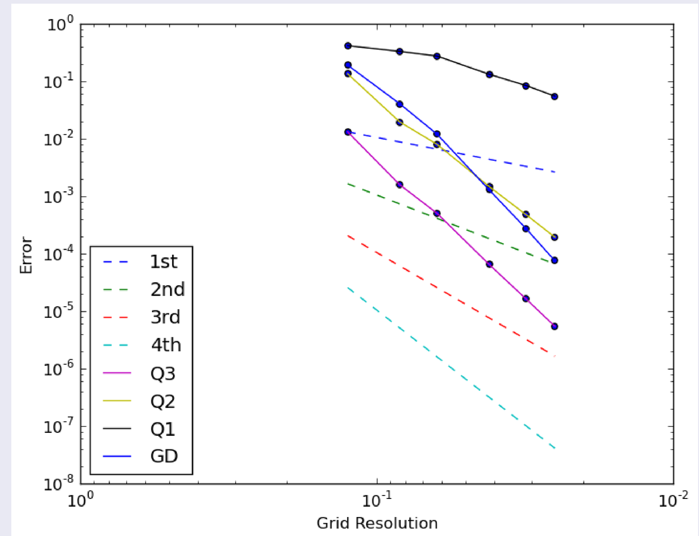
Doubly periodic boundaries on $[0,1]^3$ using a uniform hexahedral grid



Mixed $H(div)$ Helmholtz Problem

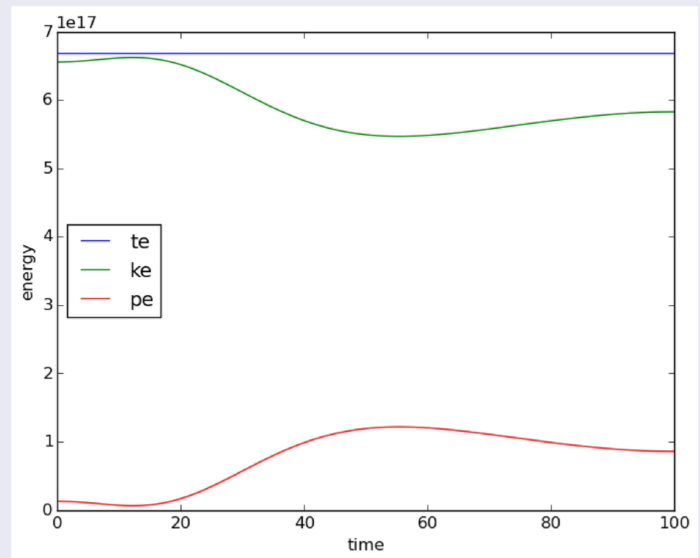
$$< \hat{h}, \vec{\nabla} \cdot \vec{u} + h > = < \hat{h}, f >$$
$$< \hat{u}, \vec{u} > + < \vec{\nabla} \cdot \hat{u}, h > = 0$$

Doubly periodic boundaries on $[0,1]^3$ using a uniform hexahedral grid



Linear Shallow Water Equations (compatible $L_2/H(div)$ spaces)

$$< \hat{h}, \frac{\partial h}{\partial t} > + H < \hat{h}, \vec{\nabla} \cdot u > = 0$$
$$< \hat{u}, \frac{\partial \vec{u}}{\partial t} + f < \hat{u}, \hat{k} \times \vec{u} >$$
$$-g < \vec{\nabla} \cdot \hat{u}, h > = 0$$



Leads to a system of equations of the form:

$$\mathrm{M} \frac{\partial \vec{x}}{\partial t} + \mathrm{S} \vec{x} = 0$$

Doubly periodic boundaries and a uniform square grid ($64x64$), initialized with a single vortex in grid center. Using implicit midpoint time stepping, energy is conserved to machine precision (assuming sufficient tolerances on linear solver).

Planned Extensions for Themis

1. New discretizations: isogeometric analysis, mimetic spectral element, Bernstein basis for $Q_r^- \Lambda^k$ family
2. Facet integrals (will enable natural boundary conditions)
3. Duality/BLAS-based assembly (see [1])
4. Integration of (a subset of) UFL and a (limited) form compiler (targeting tensor product and duality/BLAS-based assembly)
5. Multi-block domains

Hamiltonian HPE in a Lagrangian Vertical Coordinate

Prognose

$$\vec{x} = (\mu, S, \vec{v})$$

using

$$\frac{d\mathcal{F}}{dt} = \langle \frac{\delta \mathcal{H}}{\delta \vec{v}} \cdot \vec{\nabla} \frac{\delta \mathcal{F}}{\delta \mu} - \frac{\delta \mathcal{H}}{\delta \vec{v}} \cdot \vec{\nabla} \frac{\delta \mathcal{F}}{\delta \mu} \rangle + \langle \frac{\vec{\nabla} \times \vec{v}}{\mu} \cdot (\frac{\delta \mathcal{F}}{\delta \vec{v}} \times \frac{\delta \mathcal{H}}{\delta \vec{v}}) \rangle +$$
$$\langle s (\frac{\delta \mathcal{H}}{\delta \vec{v}} \cdot \vec{\nabla} \frac{\delta \mathcal{F}}{\delta \mu} - \frac{\delta \mathcal{H}}{\delta \vec{v}} \cdot \vec{\nabla} \frac{\delta \mathcal{F}}{\delta \mu}) \rangle + \langle \frac{\delta \mathcal{F}}{\delta z} \frac{\partial z}{\partial t} \rangle$$

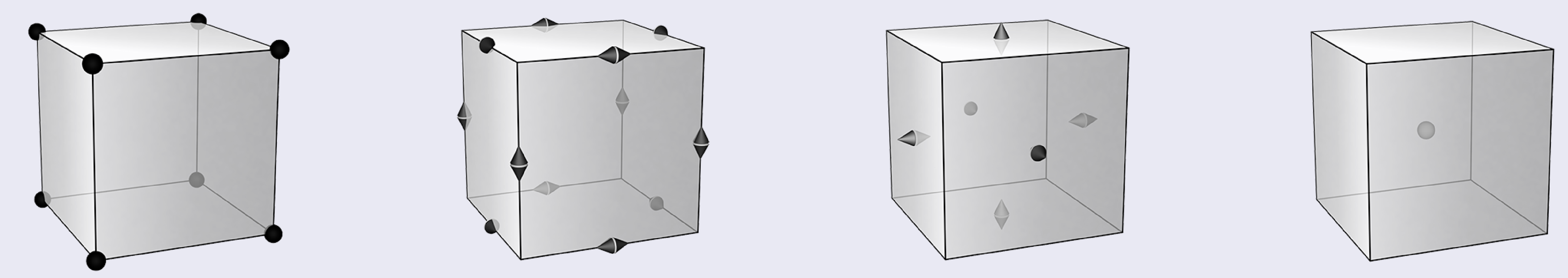
with Hamiltonian $\mathcal{H}$

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

where $\vec{u} = \vec{v} - \vec{R}$ and $S = \mu s$. Note that the brackets are 2D- vertical coupling is induced only through $\mathcal{H}$. Hydrostatic balance (which is an equation for z) is defined through $\frac{\delta \mathcal{H}}{\delta z} = 0$. Energy is conserved solely due to anti-symmetry of brackets (and $\frac{\delta \mathcal{H}}{\delta z} = 0$). See [4] for more details.

FE Spaces and Discretization

Discretization is done by restricting brackets and $\mathcal{H}$ to (appropriate) discrete subspaces, and then letting $\mathcal{F} = \int \hat{\mu} \mu d\Omega$ (or equivalent for other variables) to recover discrete weak form equations. Differential geometry says spaces and staggering should be chosen as:



$\psi \in H^1$ $\quad$ $\vec{\zeta} \in H(curl)$ $\quad$ $\vec{u}, \vec{v} \in H(div)$ $\quad$ $\mu, \delta, \chi \in L_2$

which corresponds to a FE version of C grid staggering.

1. Where should S be staggered (H^1 = differential geometry, L_2 = Lorenz, $H(div)_{vert}$=Charney Phillips)? What about auxiliary thermodynamic quantities (such as s,p,α,π)?
2. How should hydrostatic balance and $\frac{\delta \mathcal{H}}{\delta S} = \pi$ be solved? Can they be done column-wise or at least horizontal layer-wise?

This approach gives a (quasi-)Hamiltonian semi-discretization that will conserve mass, entropy and total energy.

References

[1] Robert C. Kirby. 2014. High-Performance Evaluation of Finite Element Variational Forms via Commuting Diagrams and Duality. ACM Trans. Math. Softw. 40

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[3] E. Kritsikis and T. Dubos. April 2014. Higher-order finite elements for the shallow-water equations on the cubed sphere, PDEs on the Sphere workshop

[4] Thomas Dubos and Marine Tort, 2014: Equations of Atmospheric Motion in Non-Eulerian Vertical Coordinates: Vector-Invariant Form and Quasi-Hamiltonian Formulation. Monthly Weather Review