A Structure Preserving Hydrostatic Model using Themis

Chris Eldred[1], Thomas Dubos[2] and Evaggelos Kritsikis[1]
[1]*LAGA, University of Paris 13* and [2]*LMD, Ecole Polytechnique*
Contact: *chris.eldred@gmail.com*

Themis: Accelerated Computational Science

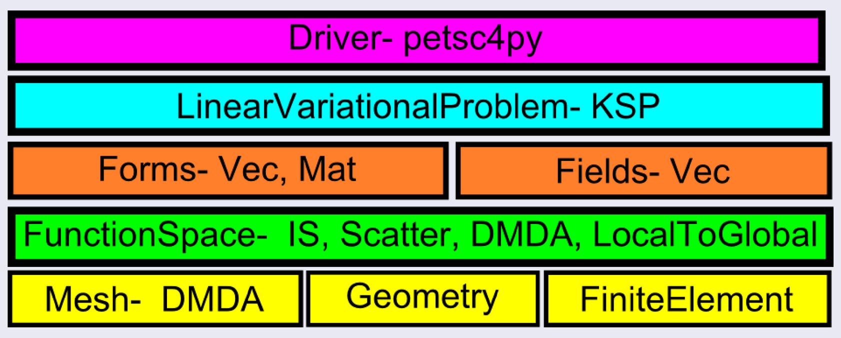
Themis is a PETSc-based software framework (written primarily in Python using petsc4py) for parallel, high-performance*, automated* discretization of variational forms (and solution of systems of equations involving them) through mimetic, tensor-product Galerkin methods. It is intended to enable a rapid 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*

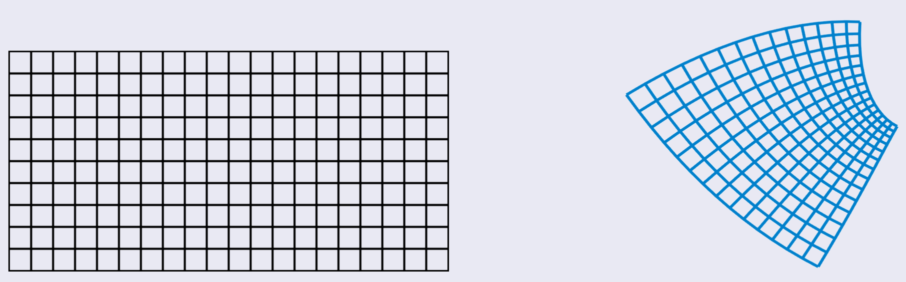
Design Principles behind Themis

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

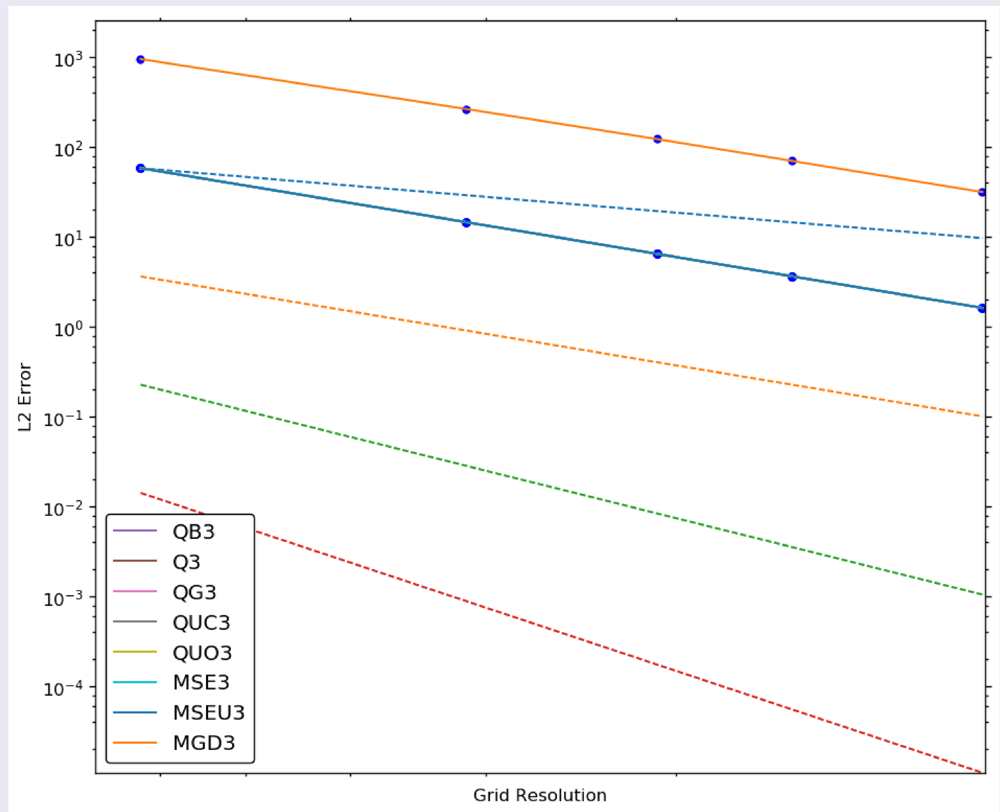
1. Support for structured grids in 1, 2 and 3 dimensions
2. Parallelism through MPI
3. Automated generation of assembly code (with user supplied kernels)
4. Arbitrary curvilinear mappings between physical and reference space
5. Support for mixed, vector and standard tensor-product Galerkin function spaces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



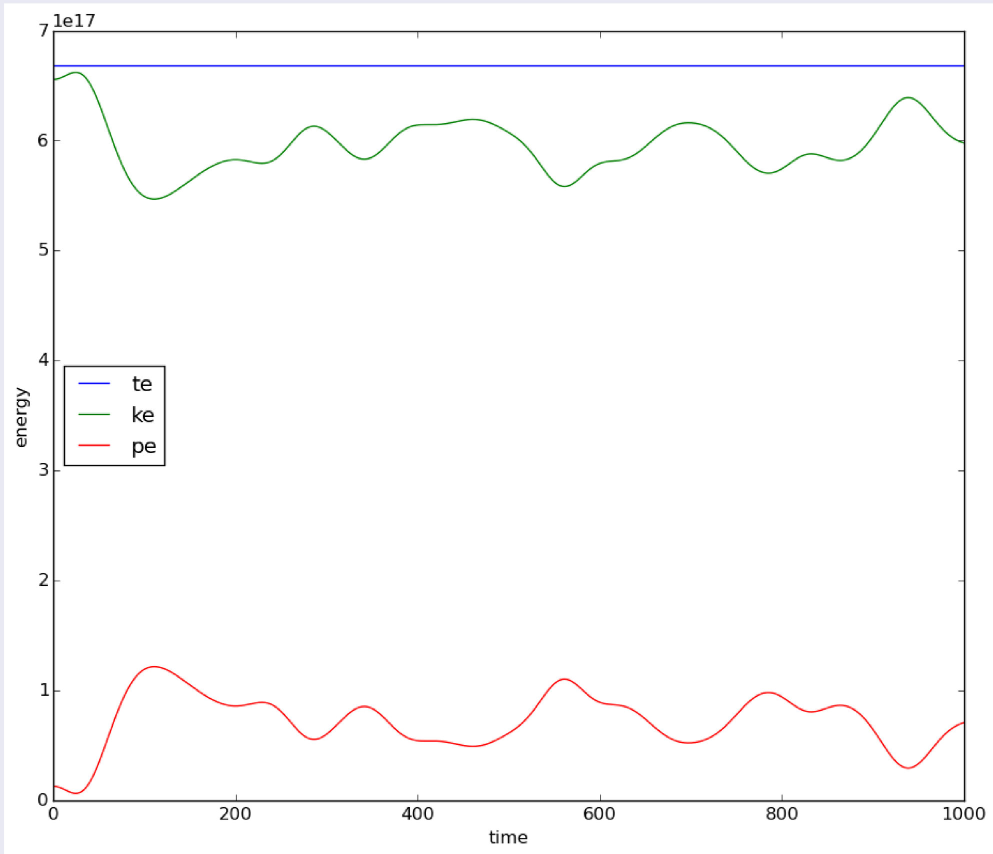
Planned Extensions for Themis

1. New discretizations: isogeometric analysis, primal-dual grid mimetic discretizations (see [4])
2. Facet integrals (will enable natural boundary conditions)
3. Duality/BLAS-based accelerated assembly
4. Integration of (a subset of) UFL and a (limited) form compiler (targeting tensor product and duality/BLAS-based assembly)
5. Multi-block domains
6. Nonlinear variational problems (via SNES)

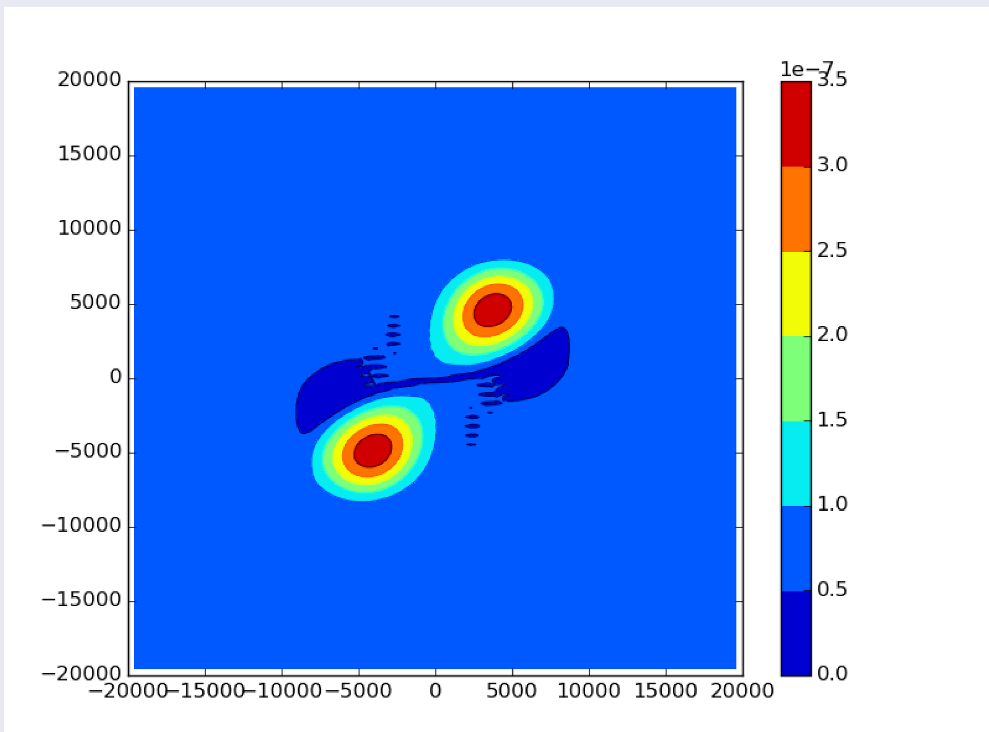
Some Results using Themis



$\boldsymbol{H(div)}$ 2D Helmholtz Problem, 3rd order, $\boldsymbol{L_2}$ error in $\vec{u}$, Uniform Grid



Linear RSWE, f-plane 3rd order MGD elements, 128x128 grid, $\boldsymbol{\Delta x \approx 40}$km, single vortex



Nonlinear RSWE, f-plane 3rd order MGD elements, 128x128 grid, $\boldsymbol{\Delta x \approx 40}$km, double vortex

General Mimetic Discretizations: Primal Grid

- Select 1D Spaces $\boldsymbol{\mathcal{A}}$ and $\boldsymbol{\mathcal{B}}$ such that: $\boldsymbol{\mathcal{A}} \xrightarrow{\frac{d}{dx}} \boldsymbol{\mathcal{B}}$
- Use tensor products to extend to n-dimensions
- All current and planned Themis discretizations fall under this framework (see [4] for more details)
- Our (novel) choices of $\boldsymbol{\mathcal{A}}$ and $\boldsymbol{\mathcal{B}}$ are guided by linear mode properties and coupling to physics/tracer transport

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

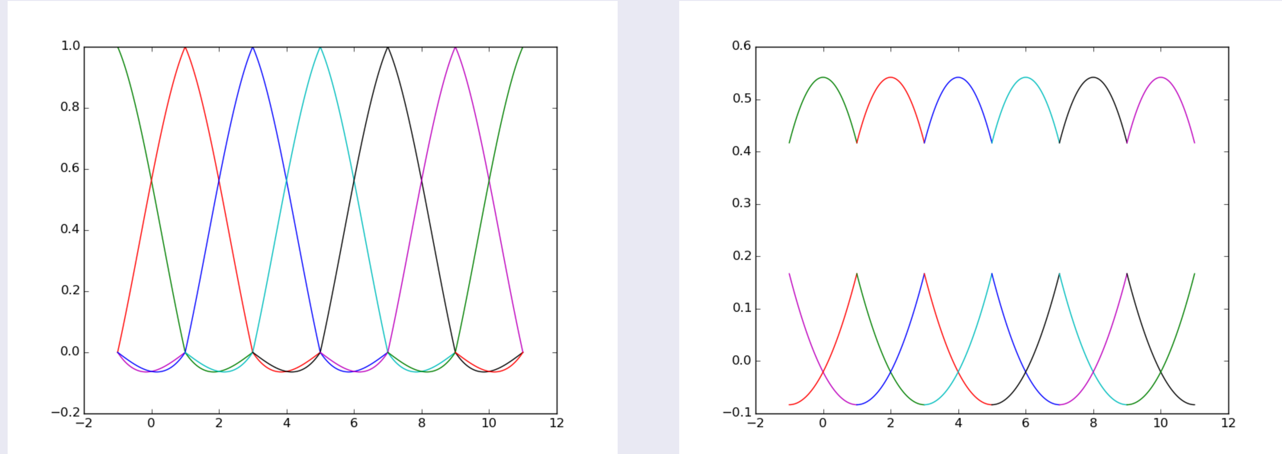
$$(da^k, b^{k+1}) = (a^k, \delta b^{k+1})$$

Primal deRham Complex

Note $\boldsymbol{\delta = *d*}$ plus integration by parts implicitly

Mimetic Galerkin Differences

$\boldsymbol{H^1}$ space defined following [1], with $\boldsymbol{L_2}$ defined to be compatible following [4]. This is an arbitrary order extension of [2]. For 3rd order gives:



$\boldsymbol{\mathcal{A} = H_1}$ Space (1D) $\qquad$ $\boldsymbol{\mathcal{B} = L_2}$ Space (1D)

Single degree of freedom per geometric entity with higher order through larger stencils $\longrightarrow$ no spectral gaps, easy coupling to physics/tracer transport, excellent wave dispersion properties, no spurious stationary modes,less local

Hamiltonian HPE in a Lagrangian Vertical Coordinate

Following [3], prognose

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

using

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

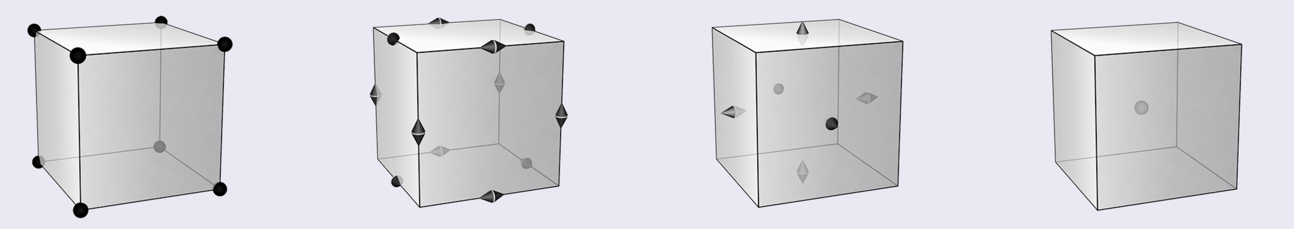
with Hamiltonian $\boldsymbol{\mathcal{H}}$

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

where $\vec{u} = \vec{v} - \vec{R}$ and $S = \mu s$. 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 $\frac{\delta \mathcal{H}}{\delta z} = 0$).

FE Spaces and Discretization

Restrict brackets and $\boldsymbol{\mathcal{H}}$ to finite subspaces, and choose $\boldsymbol{\mathcal{F} = \int \hat{\mu} \mu d\Omega}$ (or equivalent for other variables) to obtain discrete weak form equations. Differential geometry says spaces and staggering should be chosen as:



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

which corresponds to a FE version of C grid staggering.

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

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

References

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

[4] R.R. Hiemstra, D. Toshniwal, R.H.M. Huijsmans, M.I. Gerritsma. High order geometric methods with exact conservation properties, Journal of Computational Physics, January 2014