Development of a Terrestrial Dynamical Core for E3SM (TDycore)

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SciDAC Project

Objective: Develop a rigorously verified, spatially adaptive, scalable, multi-physics dynamical core for global-scale modeling of three-dimensional processes in the land component of E3SM.

Starting Point: Steady flow in porous media,

$$\mathbf{u} = -K\nabla\, p$$
$$\nabla \cdot \mathbf{u} = f$$

Two-point flux

1D currently used in Earth system models, also widely used in subsurface simulation codes.

Advantages:

- Intuitive and simple to implement
- Computationally inexpensive

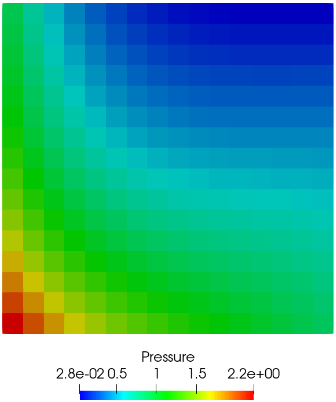
Disadvantages:

- Requires grid regularity for convergence
- Cannot handle anisotropy
- Velocity convergence is only $\mathcal{O}(h)$

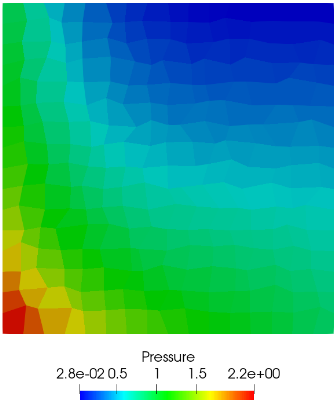
Two-point flux deficiencies

Solve a test problem, scalar permeability, perturb interior vertices by δ.

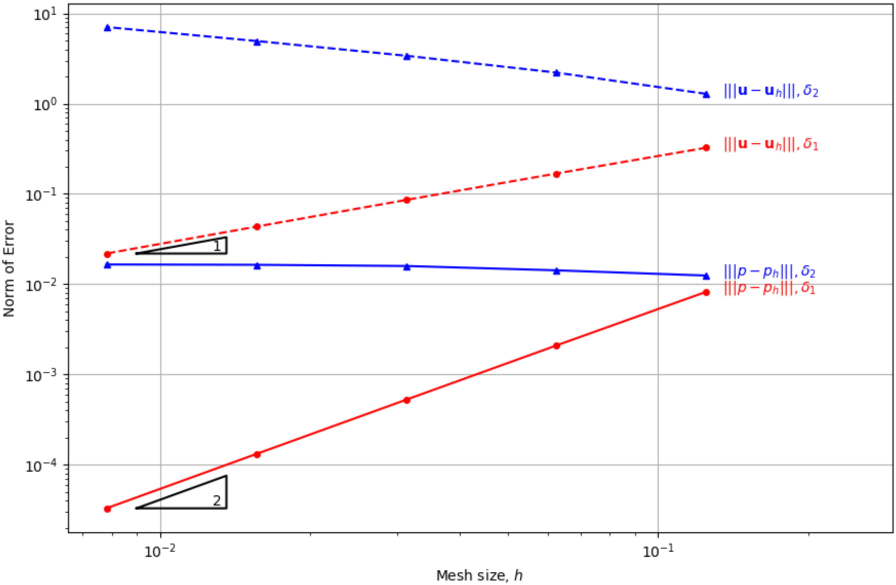
$\delta_1 = 0$



$\delta_2 = \frac{h\sqrt{2}}{3}$



Two-point flux deficiencies



Mixed finite elements with $H(\mathrm{div})$ spaces

Advantages:

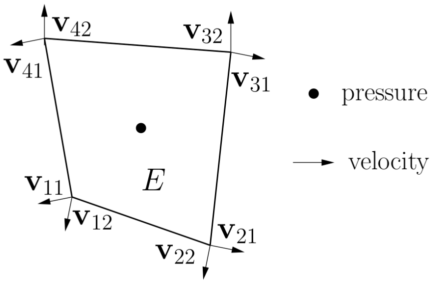
- Handles anisotropy and discontinuous coefficients
- Velocity converges at $\mathcal{O}(h^2)$
- Locally conservative

Disadvantages:

- Much more complicated, not simple finite elements
- Systems are 4x larger: include pressure and each velocity component
- Leads to a saddle-point problem

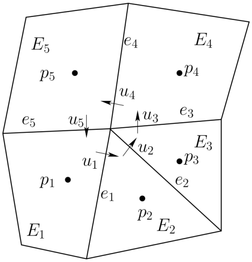
Candidate: Wheeler-Yotov

- Series of papers since 2006, designed for subsurface problems
- Wheeler, Yotov, *A Multipoint Flux Mixed Finite Element Method*, SIAM J. Numer. Anal., 44(5), 2082–2106. (25 pages)
- Constant pressure, BDM1 for velocity
- Normal component of the velocity is linear along the edge/face

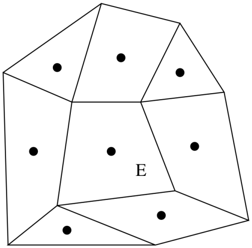


Candidate: Wheeler-Yotov

- Weak form is under-integrated using vertex quadrature
- Means that at a vertex, the velocity degrees interact only with each other and shared cell pressures
- Assembling the Schur complement leads to a cell-centered pressure stencil (27 point)

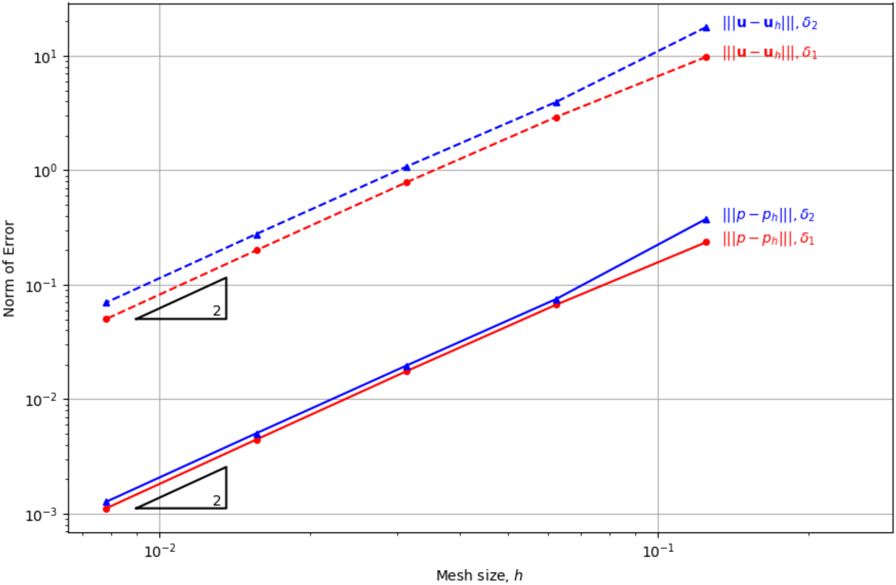


A. Five elements sharing a vertex.



B. Pressure stencil.

Wheeler-Yotov convergence



Other $H(\mathrm{div})$ discretizations/solvers

Wheeler-Yotov looks promising, but there are other options.

- Accurate quadrature BDM1 spaces: Wheeler-Yotov optimization could be suboptimal in some cases.
- Locally enriched spaces: ABF (Arnold, Boffi, & Falk, 2005) may be more accurate than Wheeler-Yotov

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These would all lead to a saddle point problem for which there are many solver options.

- Use PETSc FieldSplit preconditioner with an approximate Schur complement and then leverage standard AMG. Results in similar sparsity as Wheeler-Yotov.
- Use PETSc linear and nonlinear Multigrid, patch smoothing possible for all discretizations, can directly smooth nonlinearity with FAS.
- Use PETSc BDDC preconditioner, directly applicable to $H(\mathrm{div})$ spaces with strong convergence guarantees.

TDycore Library

We need a flexible system that can easily change discretizations as real-world comparison is crucial.

- Created TDycore: a PETSc-like C-library

  `https://github.com/TDycores-Project/TDycore`

- Written dimension/topology independent using `DMPlex` and `Section`
- Currently support quad/hex meshes in any format PETSc can read
- Ties us into full range of PETSc's solvers
- Method changable at runtime: `-tdy_method` {`tpf|wy|bdm|...`}
- Parallel development on discretization and transient nonlinear problems