Choosing a Numerical Methods for a Terrestrial Dynamical Core for the E3SM

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Method Requirements

The terrestrial water cycle is a key component of the Earth system model, yet while conceptually key processes transport water laterally, the representation is 1D in current models. We aim to identify and implement a numerical method which satisfies the following requirements:

- Accurate velocities on distorted grids
- Due to uncertain parameters, low order pressure is sufficient
- Target method should exhibit good strong scaling

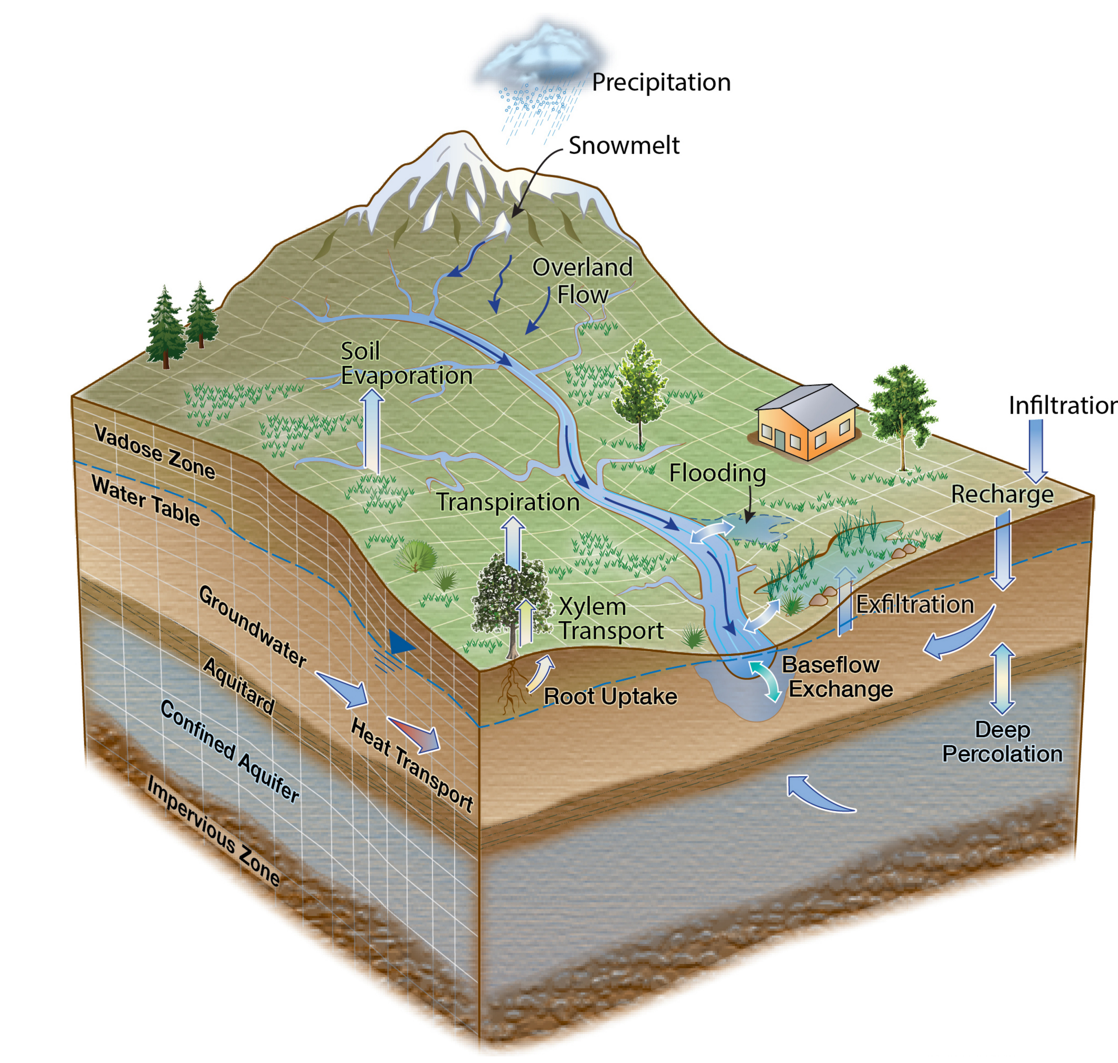


Figure 1: Schematic of important hydrological processes in Earth system models

Initially, we will pare down the full system to study computational efficiency/scalability of the spatial operator.

Strong form Find $\mathbf{u}$ and p such that,

$$\begin{aligned} \mathbf{u} &= -K\nabla p && \text{in } \Omega \\ \nabla\cdot\mathbf{u} &= f && \text{in } \Omega \\ p &= g && \text{on } \Gamma_D \\ \mathbf{u}\cdot\mathbf{n} &= 0 && \text{on } \Gamma_N \end{aligned}$$

Weak form Find $\mathbf{u} \in \mathbf{V}$ and $p \in W$ such that,

$$\begin{aligned} \left(K^{-1}\mathbf{u},\mathbf{v}\right) &= \left(p,\nabla\cdot\mathbf{v}\right) - \langle g, \mathbf{v}\cdot\mathbf{n}\rangle_{\Gamma_D}, && \mathbf{v}\in\mathbf{V} \\ \left(\nabla\cdot\mathbf{u}, w\right) &= \left(f, w\right), && w \in W \end{aligned}$$

where $\mathbf{V} = \{\mathbf{v} \in H^{\text{div}}(\Omega) : \mathbf{v}\cdot\mathbf{n} = 0 \text{ on } \Gamma_N\}$, $W = L^2(\Omega)$

Possible Method Families

- **Finite volume methods**: traditional two-point flux lacks geometric flexibility, low flux accuracy, other methods address these weaknesses (Multi-point flux approximation: O-method (MPFA-O))
- **Continuous Galerkin finite elements**: lack local conservation despite conceptual simplicity and fewer unknowns, reduced flux accuracy, create artifacts deadly for nonlinear problems (not considered)
- **Discontinuous Galerkin finite elements**: locally conservative but no continuity in the flux, lower flux accuracy than in mixed finite elements, proliferate in numbers of unknowns (not considered)
- **Mixed finite elements**: approximate the primal variable and flux simultaneously using finite element pairs that satisfy the inf–sup condition. But the resulting indefinite linear systems (saddle-point problems) require special solvers (Brezzi–Douglas–Marini (BDM), Wheeler-Yotov (WY), Arnold-Boffi-Falk (ABF))

Mixed Finite Elements: BDM

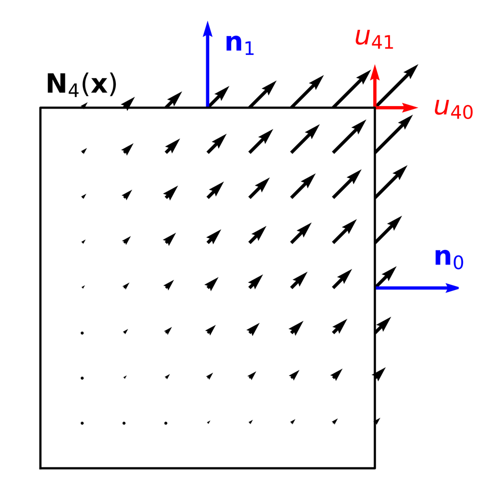
Mixed finite element discretizations lead to saddle-point problems of the type:

$$\begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} U \\ P \end{bmatrix} = \begin{bmatrix} G \\ F \end{bmatrix}$$

which we solve using the physics-based preconditioning methods implemented into PETSc's `fieldsplit`. While intuitively this larger system should cost more to solve than that of pressure only, in practice this is not always true. It may also be that enriched spaces (such as ABF) could provide better accuracy for marginal increases to solvers and be a better option.

Wheeler-Yotov (WY)

In (Wheeler & Yotov, 2006) the authors develop a mixed finite element method that reduces to cell-centered finite differences on quadrilateral and simplicial grids and performs well for discontinuous full tensor coefficients.



Ingredients:

- Brezzi–Douglas–Marini (BDM_1) velocity space
- Basis interpolatory at corners
  $\mathbf{N}_4(\mathbf{x}_4)\cdot\mathbf{n}_0 = u_{40}$
  $\mathbf{N}_4(\mathbf{x}_4)\cdot\mathbf{n}_1 = u_{41}$
- Vertex-based quadrature
- Constant pressure space

This means that velocity DOFs only couple to each other at vertices and allows for local elimination. This leads to a symmetric positive definite system in terms of pressures on which we can use algebraic multigrid.

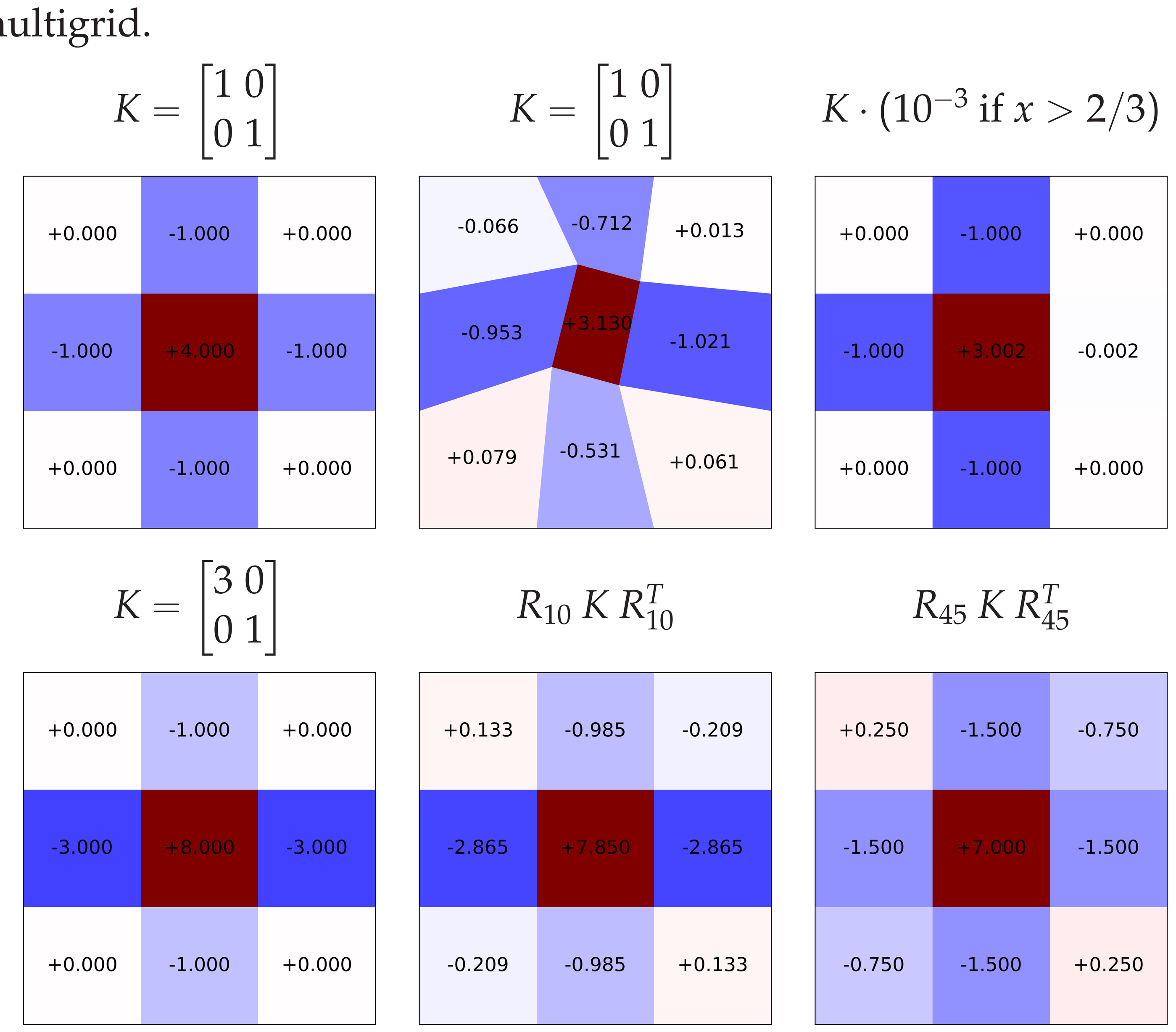


Figure 2: Sample WY stencils. Under sufficient conditions, the stencil reduces to that of finite differences. The WY methodology gives us a variationally consistent way to derive stencils as parameters change.

SPE10 Test Problem

As an initial stress test, we use the permeability from the SPE10 problem:

- $60 \times 220 \times 85 = 1{,}122{,}000$ cells
- Diagonal permeability $K_{xx} = K_{yy} \neq K_{zz}$
- We induce flow by Dirichlet conditions
- Solve on original permeability and also rotate around two axes

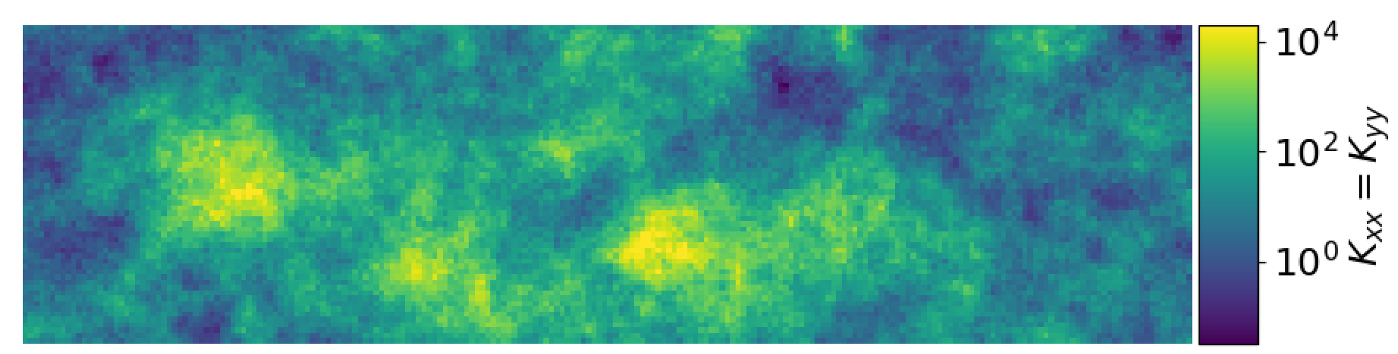


Figure 3: Sample slice of the permeability field

We solve the SPE problem on Cori-Haskell and show strong scaling results in Figure 4. While still a work in progress, we notice the following from these results:

- WY (blue) is the most robust approach, it scales well for both the diagonal and full tensor permeability. For the diagonal problem, its performance is equivalent to the two point flux method with harmonic averaging of the permeability.
- Performance of the BDM method with depends heavily on the parameters of `pcfieldsplit`. Solving using GMRES with CG/jacobi+CG/HYPRE (green) is accurate, but hits the strong scaling limit quickly.
- If we loosen `fieldsplit` parameters and use `preonly` in place of CG (red), performance is much better without a decline in accuracy
- None of the BDM methods work on the tensor problem with the default PETSc options, we are working on a more specialized option using the WY matrix to precondition the pressure system.

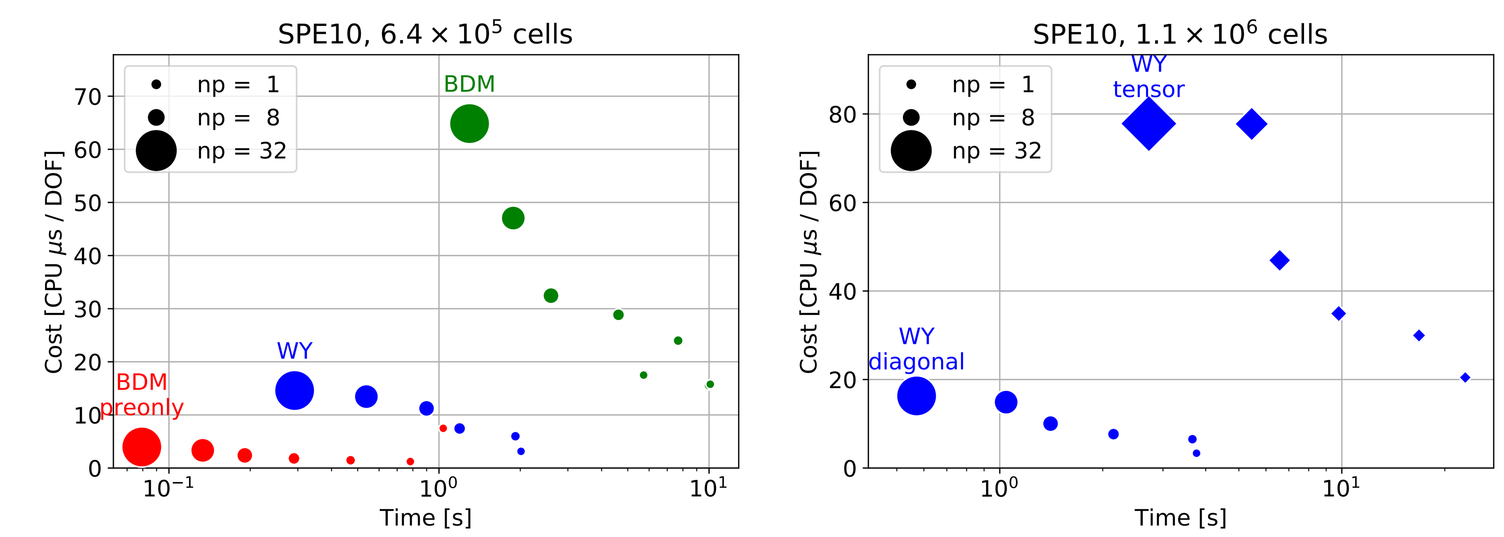


Figure 4: (left) SPE10 diagonal permeability problem on a smaller grid such that all methods can run (right) SPE10 tensor permeability, WY/AMG is the only method which solved

Important Information

This work has been implemented into a C-library based heavily on PETSc, using not only their solvers but also the `Plex` and `Section` to implement the discretizations. While written in C, we have FORTRAN interfaces. The codebase is developed openly and available here:

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

This work is supported by the U.S. Department of Energy, Office of Science, Office of Biological and Environmental Research, and Office of Advanced Scientific Computing Research Scientific Discovery through Advanced Computing (SciDAC) program under Contract No. DE-AC05-76RL01830.