Development Plans for the Subsurface Terrestrial Dynamical Core of E3SM

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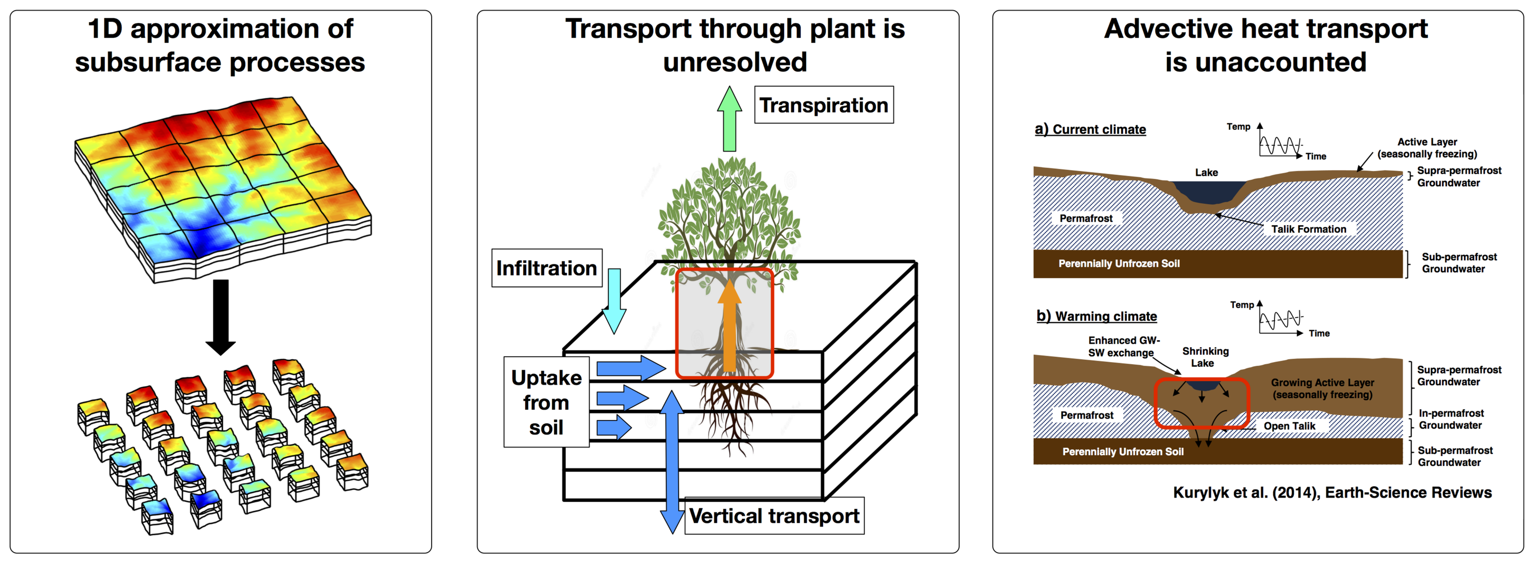
Motivation

- Developing a predictive understanding of the terrestrial water cycle at local to global scale is essential for accurate assessment of water resources, agricultural production, and energy generation given current climate variability.
- Terrestrial component of the U.S. Department of Energy's (DOE's) E3SM excludes many critical physical processes



- Due to missing process representations, E3SM is unable to answer following key research questions:
  - How topography may mitigate drought effects on vegetation along a hillslope gradient?
  - How hydraulic functional traits of root, stem, and leaf will determine the response of tree to future drought in presence of topographic gradients?
  - Will inclusion of advective energy transport significantly alter prediction of permafrost thaw?
- Computational challenges associated with E3SM's 10-year vision of resolving terrestrial processes at sub-kilometer resolution include:
  - Solving nonlinear parabolic PDEs with approximately 10 billion unknowns
  - Using spatial discretization of PDEs that account for non-orthogonal grids
  - Flexibility to solve tightly coupled multi-component, multi-physics problems

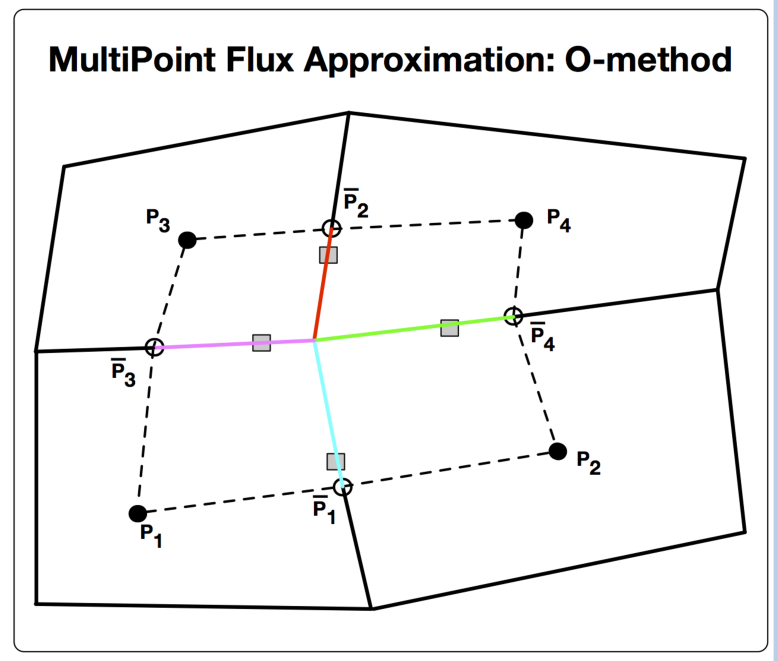
Objectives

- In Phase-I of this project, we will develop a rigorously verified, spatially adaptive, scalable, multi-physics dynamical core (dycore) for global-scale modeling of three-dimensional subsurface processes
- The dycore will use the Portable, Extensible Toolkit for Scientific Computation (PETSc) library to provide numerical solution of discretized equations

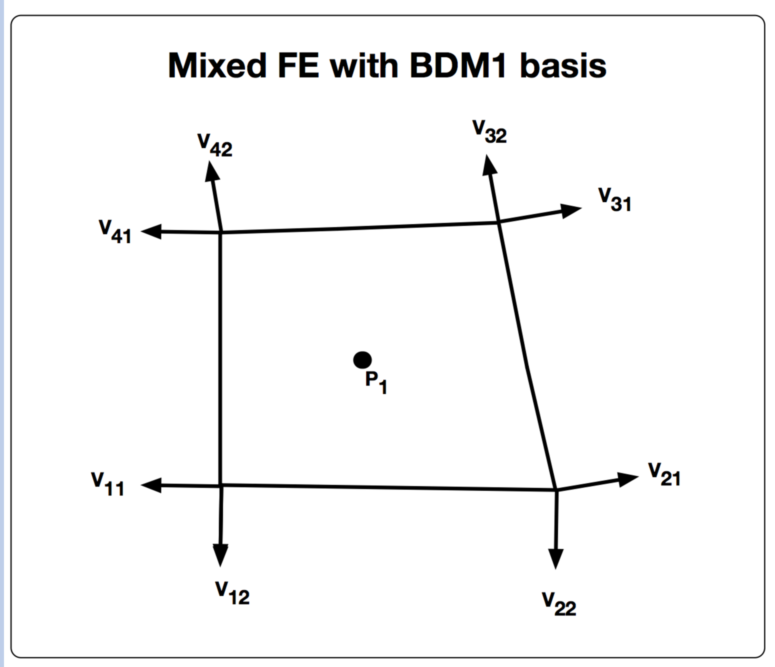
Spatial Discretization: Methods

- High spatial resolution in complex terrain leads to non-orthogonal three dimensional grids
- Two spatial discretization methods have been identified that account for non-orthogonal grids and have been previously applied to solve for subsurface flow and transport processes

1. **M**ulti **P**oint **F**lux **A**pproximation (MPFA) - O method
   - Based on finite volume in which control volumes are subdivided into interaction volumes (IVs)
   - Pressure varies linearly and flux continuity is enforced across IVs
   - Discretization can be performed in physical or reference space
   - Number of unknowns are cell-centered pressure values



2. **M**ixed **F**inite **E**lement (MFE) method



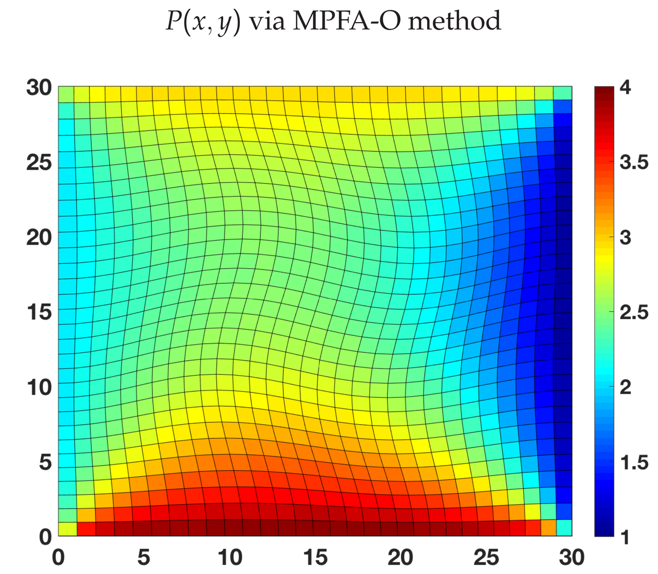
- BDM1 basis assumes that normal velocity may vary linearly along a edge
- Discretization is performed in a reference space
- Choice of numerical quadrature reduces the number of unknowns to cell centered pressure values

- MPFA-O and MFE methods have different error convergence properties for rough grids

Spatial Discretization: Results

- Developed a prototype code for solving 2D steady-state diffusion equation using MPFA-O method
  - Solves $\nabla \cdot (K \nabla P) = 0$ on a 2D non-orthogonal grid with $K = 1$, $P_{south} = 4$, $P_{north} = 3$, $P_{right} = 1$, and $P_{left} = 2$
  - Preliminary comparison of our results show good agreement with the MATLAB Reservoir Simulation Toolbox

$P(x, y)$ via MPFA-O method

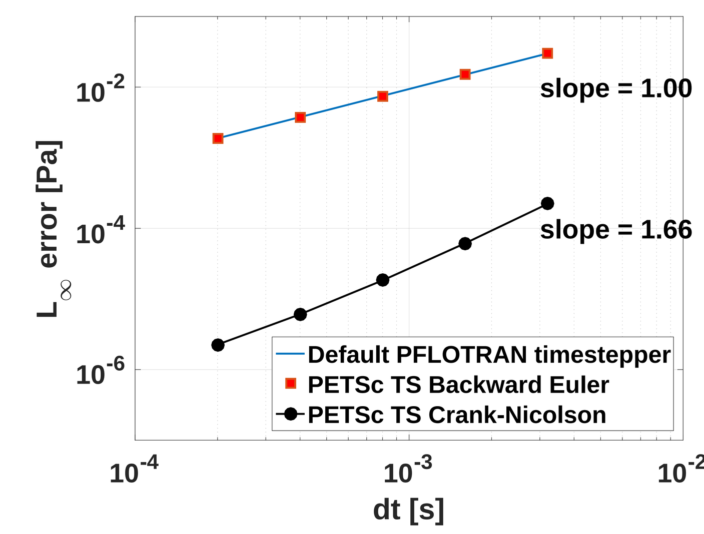


Temporal Discretization: Methods

- The dycore will use PETSc time-stepper (TS) for temporal discretization
- Use of TS will enable easy experimentation with multiple time integration algorithms and allow the development of an adjoint model in the future for data assimilation

Temporal Discretization: Results

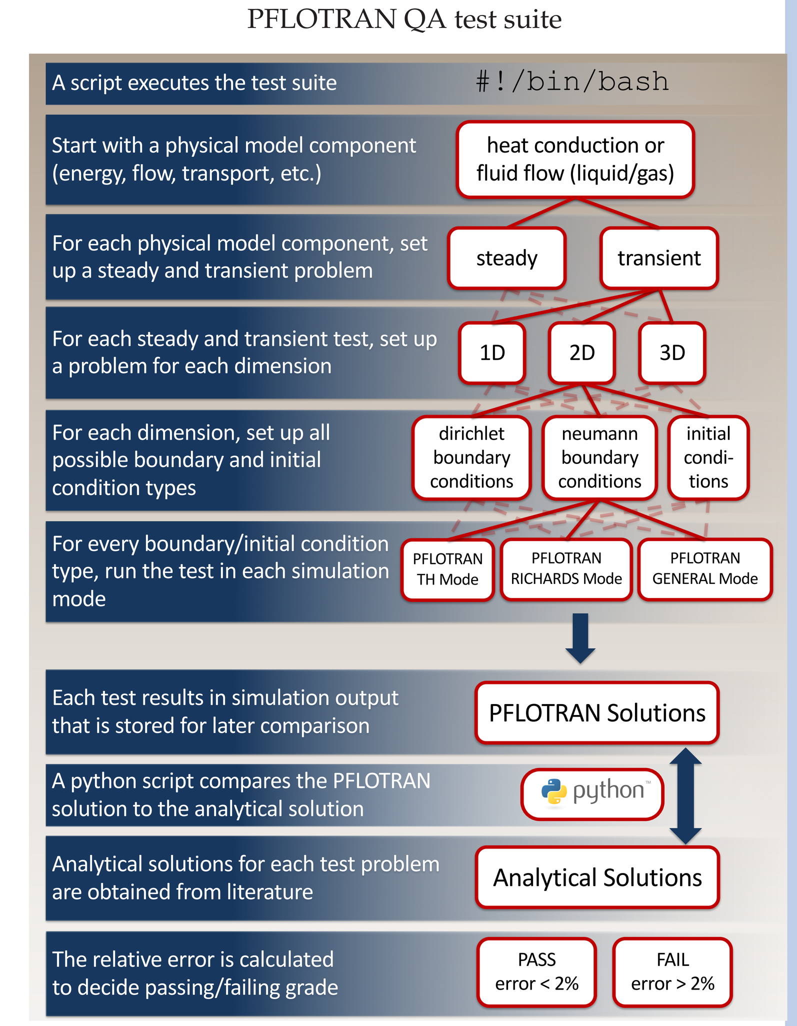
- Implemented PETSc TS based solver in PFLOTRAN, a subsurface flow and transport model that uses first-order spatial discretization
- Error convergence study is performed for a 1D soil column problem in which liquid pressure evolves towards a hydrostatic equilibrium starting with a spatially homogenous initial condition
  - Error for the default PFLOTRAN timestepper and TS backward Euler converges at the same expected rate
  - Error for TS Crank-Nicolson converges at a higher rate that TS backward Euler



Next steps

- Extend prototype codes for MPFA-O and MFE methods to support 3D problems
- Study error convergence for MPFA-O and MFE for non-orthogonal grids
- Develop a verification and validation test suite for the dycore
- Apply the dycore for a range of terrestrial multi-physics problems at global scales

PFLOTRAN QA test suite



Acknowledgements

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