Development of Terrestrial Dynamical Core for the E3SM to Simulate Water Cycle

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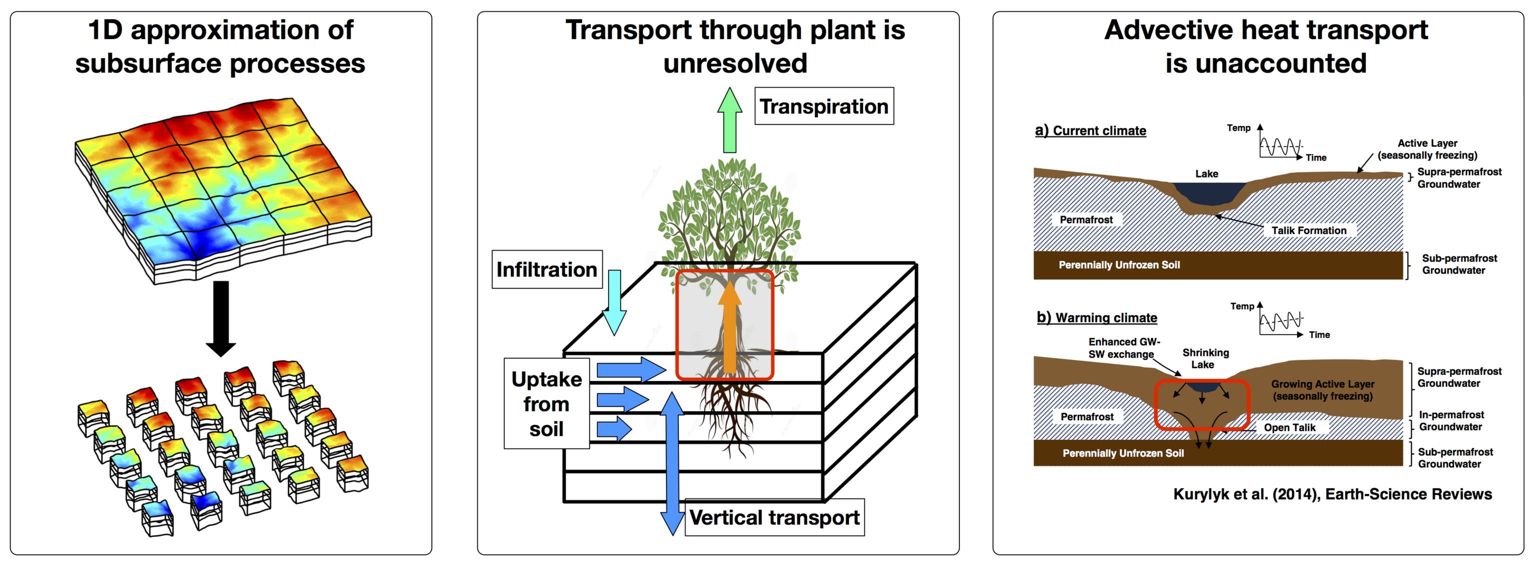
Motivation

- 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 DOE's E3SM excludes many critical physical processes:



Objective

- Develop a rigorously verified, spatially adaptive, scalable, multi-physics dynamical core for global-scale modeling of three-dimensional subsurface processes for E3SM

Terrestrial Dynamical core

The **T**errestrial **Dy**namical **core** (TDycore) will solve 3D transport of water and energy in the subsurface given by:

$$\frac{\partial}{\partial t}(\rho\phi s) = -\nabla\cdot(\rho\mathbf{q}) + Q_w \quad (1)$$

$$\frac{\partial}{\partial t}(\rho\phi s U + (1-\phi)\rho_p C_p T) = -\nabla\cdot(\rho\mathbf{q}H - \kappa\nabla T) + Q_e \quad (2)$$

where $\mathbf{q} = \frac{k_r K}{\mu}\nabla(P + \rho g z)$

We are pursuing a two pronged development that is focused on:

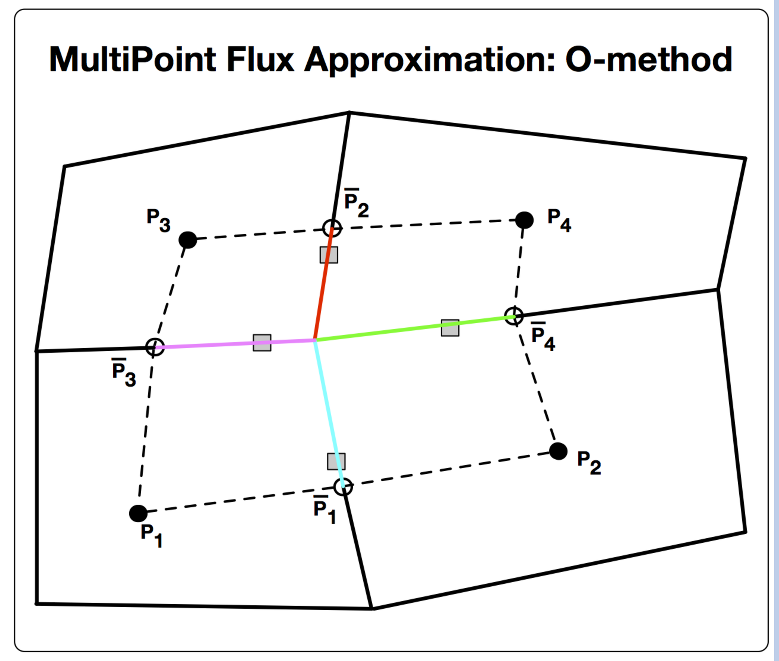
1. Using spatial discretization methods that accounts for non-orthogonal grids
2. Using a flexible framework that supports with different temporal discretization schemes

Development of TDycore library

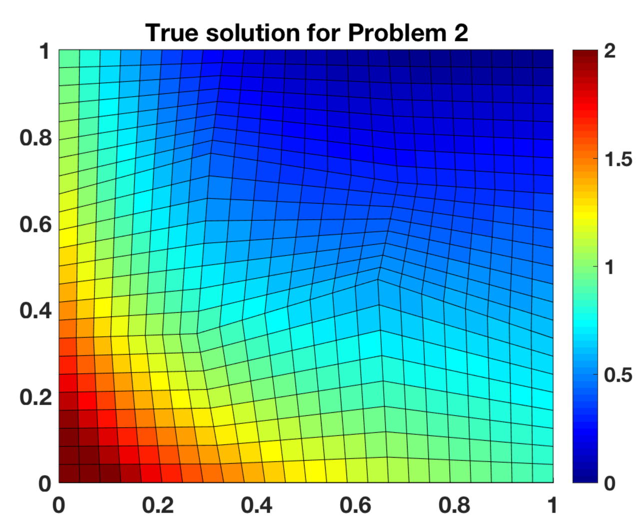
- Developing a scalable *library* on top of PETSc framework
- E3SM terrestrial dycore will be an application of the TDycore library
- Open-source and open-development
- Core library is written **in C with Fortran bindings**
- Supports runtime configurability: `-tdy_method {wy|mpfao|...}`
- Using a modified PFLOTRAN's regression testing framework
- Includes 5 demo applications and 27 regression tests
- Available on Github: `https://github.com/TDycores-Project/TDycore`
- Using Travis-CI for regression testing `https://travis-ci.org/TDycores-Project/TDycore`
- Regression tests cover 95% of the code `https://codecov.io/gh/TDycores-Project/TDycore`

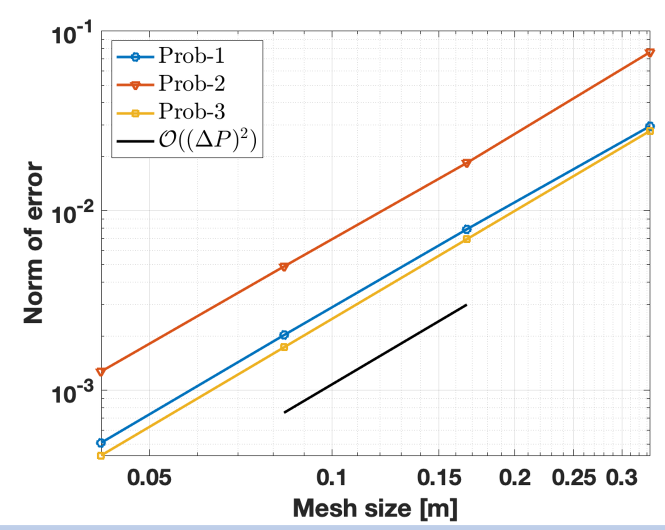
Multi Point Flux Approximation: O-method

- 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
- Method of Manufactured Solutions is used to verify the serial implementation

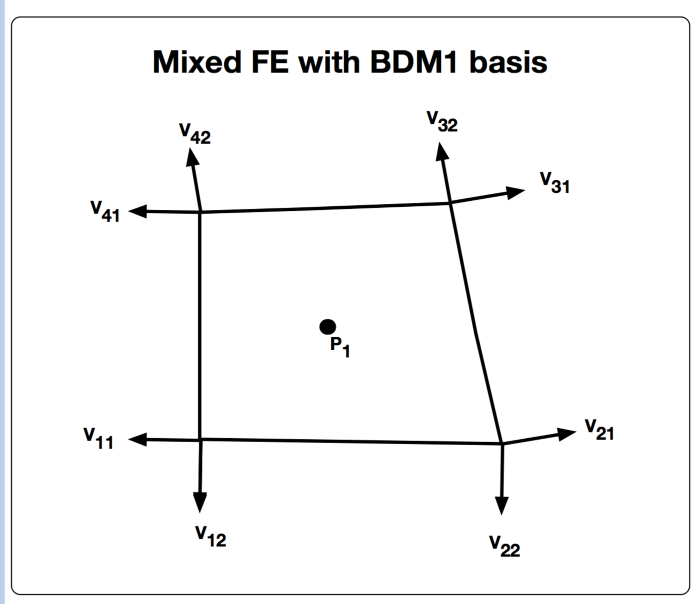


1. $P = 3.14 + x(1-x) + y(1-y)$ and $K_{11} = 5$; $K_{22} = 2$; $K_{12} = K_{21} = 1$
2. $P = (x-1)^4 + (1-x)(1-y)^3 + \sin(1-y)\cos(1-x)$ and $K_{11} = 5$; $K_{22} = 2$; $K_{12} = K_{21} = 1$
3. $P = x(1-x) + y(1-y) + z(1-z)$ and $K_{11} = 5$; $K_{22} = 2$; $K_{33} = 3$ and $K_{ij} = 1$ for $i \neq j$





Mixed Finite Element

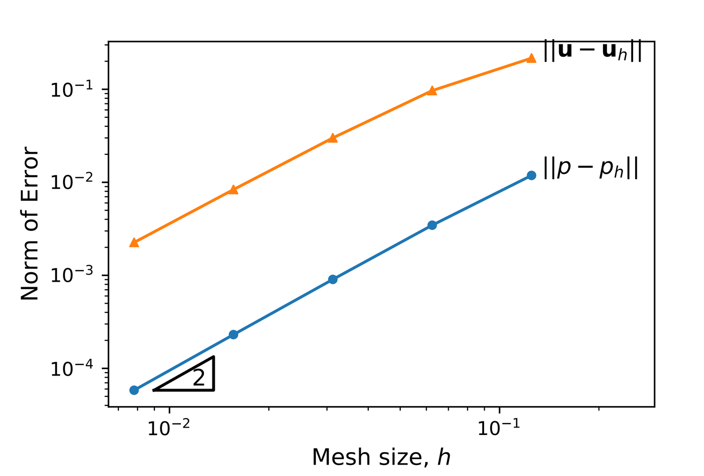


- Handles discontinuous coefficients on non-orthogonal grids
- BDM1 basis assumes that normal velocity may vary linearly along a edge and pressure is constant
- Leads to a saddle point problem that requires specialized preconditioning techniques
- Also implemented Wheeler-Yotov (WY) method,

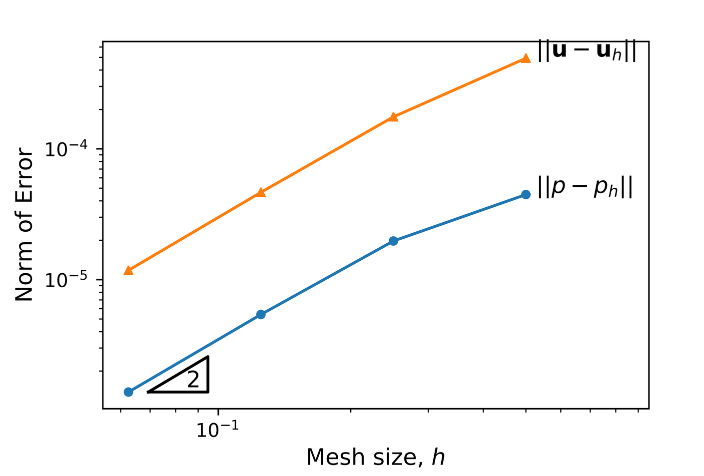
which uses special quadrature to allow for local velocity elimination

- WY leads to a symmetric and positive definite cell-centered system for pressure unknowns
- Implemented and tested for distorted 2D and 3D grids in parallel

Problem 2

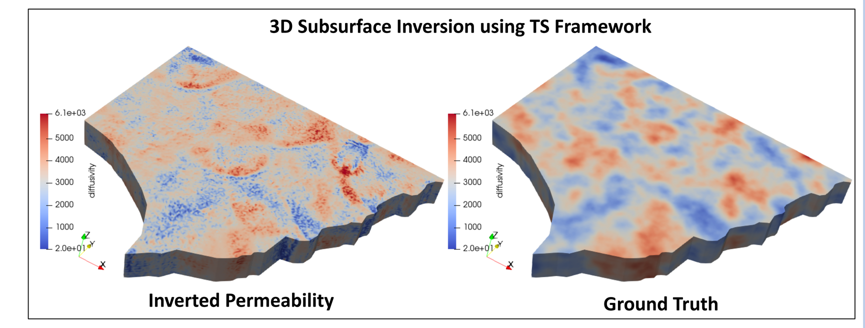


Problem 3



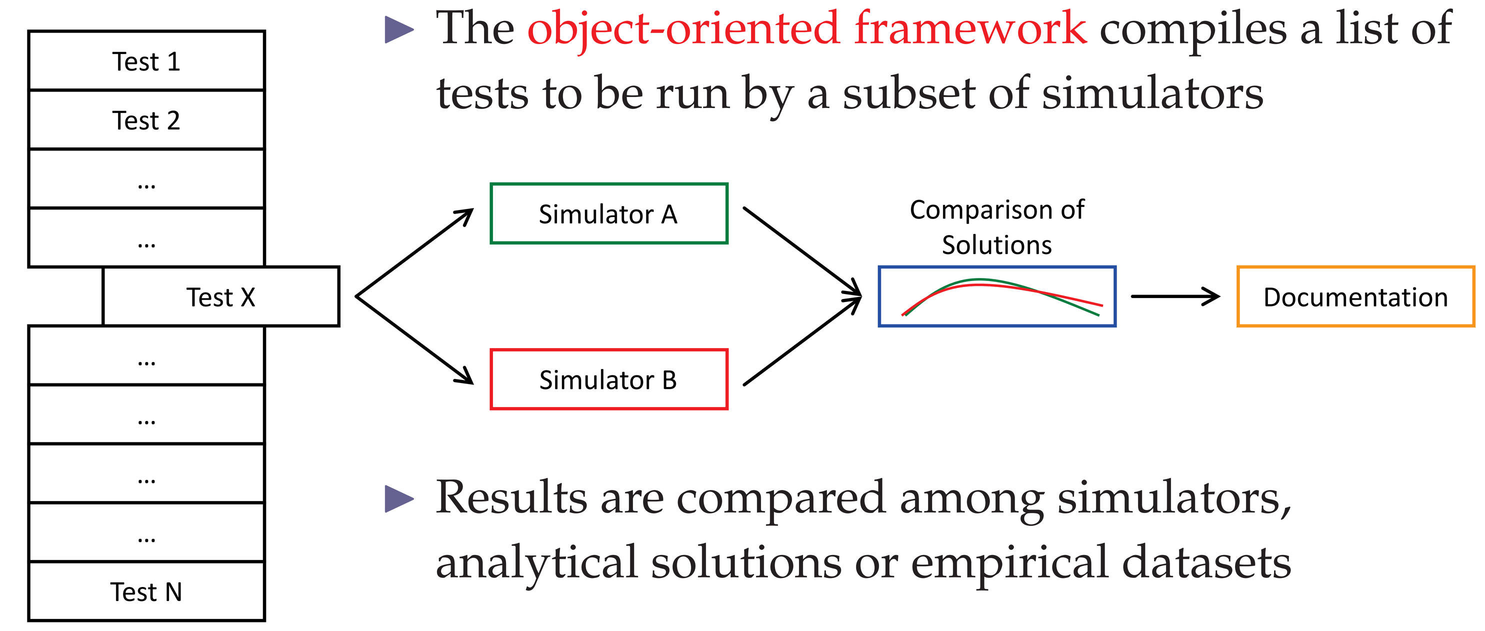
Temporal discretization: Methods

- Implemented and tested flexible temporal discretization framework, PETSc TS, for the mass and energy subsurface governing equations
- Allows to choose from 12 types of time integrators (e.g., Backward Euler, Crank-Nicholson, Theta, etc.) on the fly without any new code development
- TS framework can be used to build discrete adjoints for sensitivity analysis and inversion with minimal code addition

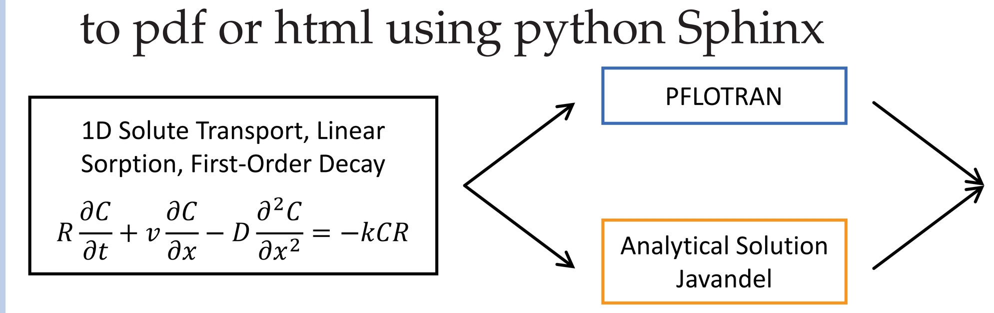


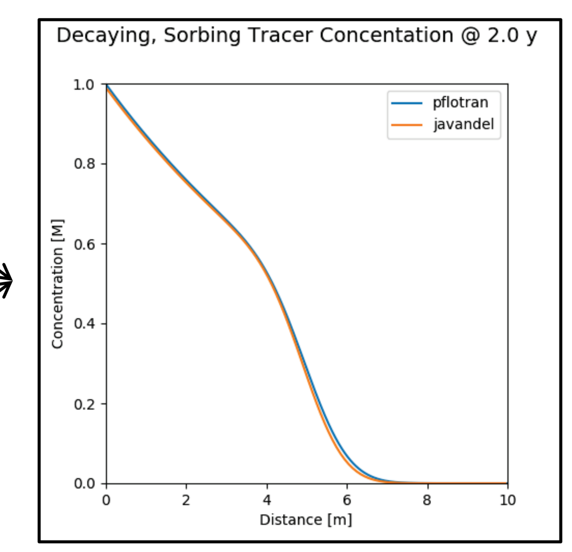
V&V framework

- Developing an automated, python-based framework for V&V testing in the cloud that is code-agnostic



- The object-oriented framework compiles a list of tests to be run by a subset of simulators
- Results are compared among simulators, analytical solutions or empirical datasets
- Documentation is generated in reStructuredText format and compiled to pdf or html using python Sphinx





Next steps

- Extend MPFA-O method to support multiple processors
- Perform an inter-comparison of spatial discretization methods
- Combine the developments in spatial and temporal discretization methods to solve a non-linear, transient subsurface flow problem on non-orthogonal grids
- Use the V&V framework to benchmark the dycore
- Couple the TDycore with ELM for watershed scale simulation

Acknowledgements

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