Development of Terrestrial Dynamical Core for E3SM

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ESMD PI Meeting
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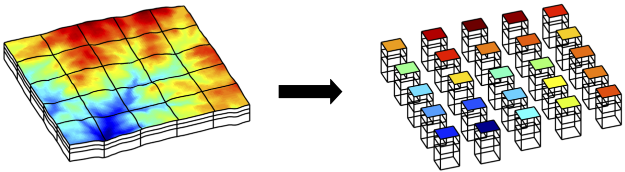
Scientific Discovery through Advanced Computing

Shortcomings of biophysical processes in ELM

- ELMv2.0 will neglect lateral transport of soil moisture and subsurface heat

1D approximation of subsurface processes



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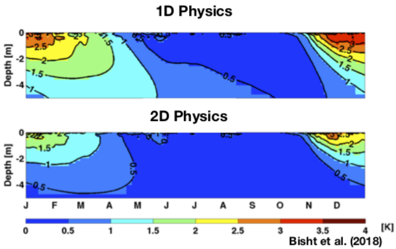
- ELMv2.0 will neglect lateral transport of soil moisture and subsurface heat
- Lateral redistribution of soil moisture leads to an increase in predicted surface energy fluxes at watershed[1] and continental scales[2]
- Lateral redistribution of subsurface heat leads to a decrease of spatial variability in soil temperature[3]



Spatial std. dev. of T_{soil} for a transect in Barrow, AK

[1]Tague and Peng, 2013; [2]Maxwell and Condon, 2016; [3]Bisht et al., 2018

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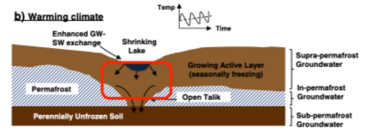
- Lateral redistribution of soil moisture leads to an increase in predicted surface energy fluxes at watershed[1] and continental scales[2]
- Lateral redistribution of subsurface heat leads to a decrease of spatial variability in soil temperature[3]
- Advective heat transport, which will not be modeled in ELMv2.0, may accelerate the rate of permafrost thaw[4]

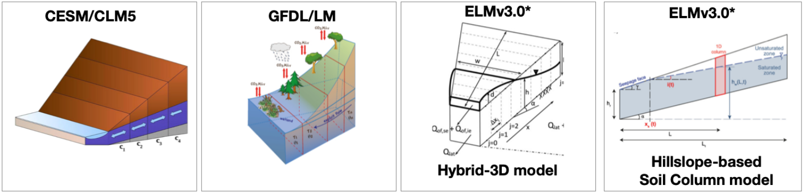


Kurylyk et al. (2014), Earth-Science Reviews

[1]Tague and Peng, 2013; [2]Maxwell and Condon, 2016; [3]Bisht et al., 2018 ; [4]Kurylyk et al. 2014

Shortcomings of biophysical processes in ELM

- A key biophysical process that has been identified for next-generation LSMs is lateral subsurface flow[1]
- Integration of conceptual models for representing a 1D hillslope within a LSM grid cell is underway.



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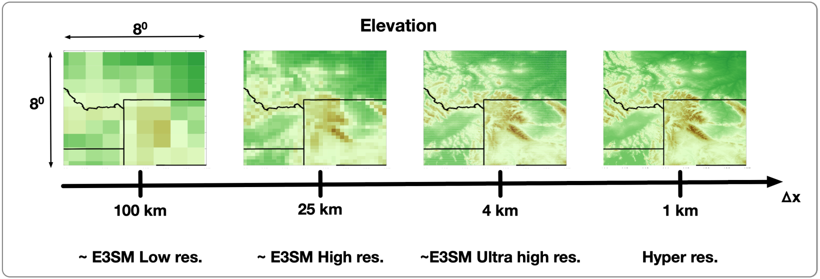
- Integration of conceptual models for representing a 1D hillslope within a LSM grid cell is underway.
- Higher horizontal resolution in future ESMs would require explicit representation of subsurface lateral processes.



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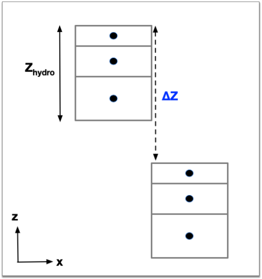
Computational challenges for ELM with 3D subsurface processes

- Need to use terrain-following grids



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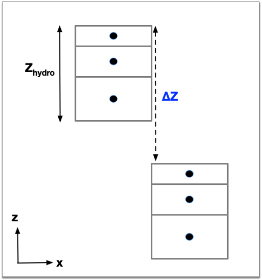

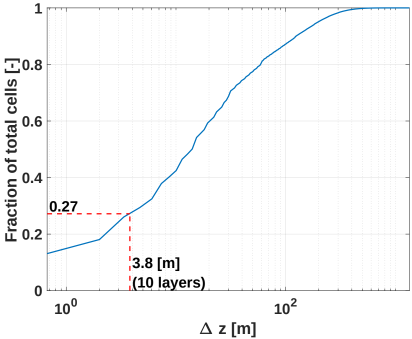

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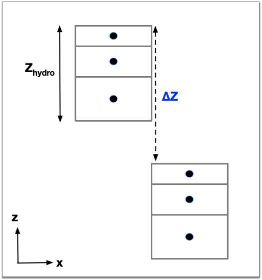
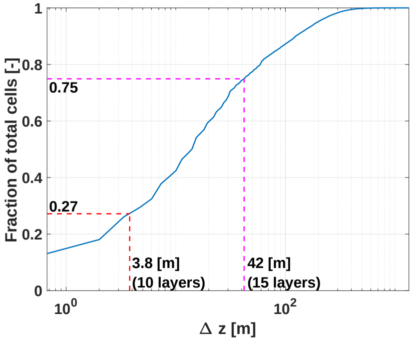
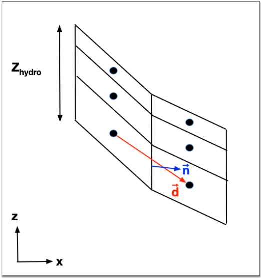
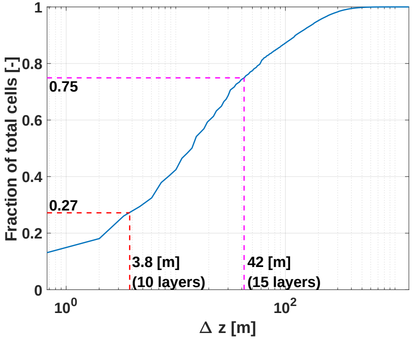




Computational challenges for ELM with 3D subsurface processes

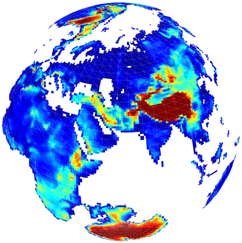
- Need to use terrain-following grids that are non-orthogonal for which low-order spatial discretization methods may not be accurate





Computational challenges for ELM with 3D subsurface processes

- Need to use terrain-following grids that are non-orthogonal for which low-order spatial discretization methods may not be accurate
- Scalable solver for nonlinear parabolic PDE with 10^{10} unknowns



Computational challenges for ELM with 3D subsurface processes

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- Scalable solver for nonlinear parabolic PDE with 10^{10} unknowns
- Need to support heterogenous computing architecture

Terrestrial Dynamical core (TDycore) library

- Developed a scalable *library* on top of PETSc framework
- Open-source and open-development
- Core library is written in C with Fortran bindings
- Supports runtime configurability: `-tdy_method {wy|mpfao|...}`
- Developed a regression testing framework for the TDycore lib
- Includes 13 demo examples and 42 regression tests
- Available at `https://github.com/TDycores-Project/TDycore`
- Using Travs-CI for regression testing
  `https://travis-ci.org/TDycores-Project/TDycore`
- Regression tests cover 85% of the code
  `https://codecov.io/gh/TDycores-Project/TDycore`

The coupled thermal-hydrology model

The TDycore will solve 3D transport of water and energy in the subsurface given by:

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

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

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

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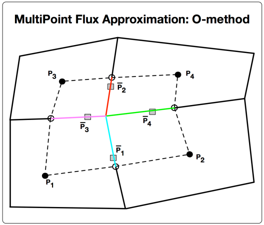
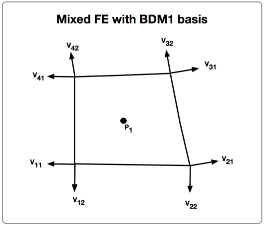
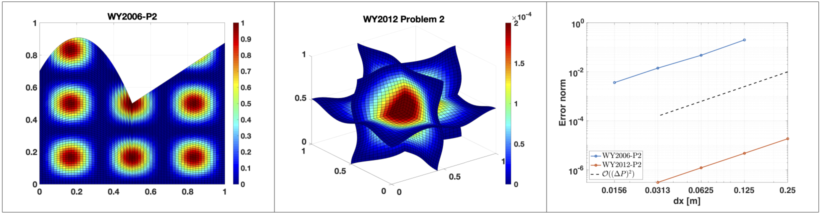
1. Using spatial discretization methods that accounts for non-orthogonal grids
2. Using a flexible framework that supports experimenting with different temporal discretization schemes

Supported discretizations

- Spatial discretizations
  - Multi-point flux approximation
  - **M**ixed **F**inite **E**lement
- Used **M**ethod of **M**anufactured **S**olutions for code verification





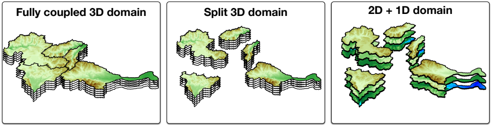


- Temporal discretizations
  1. Hard-coded backward Euler
  2. PETSc **T**ime **S**tepper[1]

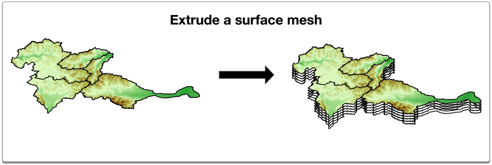
[1] Contributed a conservative time integration scheme to PETSc.

TDycore meshes

- Support multiple mesh configurations

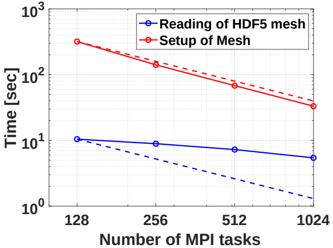


- Input mesh types: (i) 3D and (ii) surface mesh that can be extruded[1]



- A surface mesh with 70×10^6 grid cells is extruded 30 soil layer deep ($= 2.1\times10^9$ grid cells)

Compy

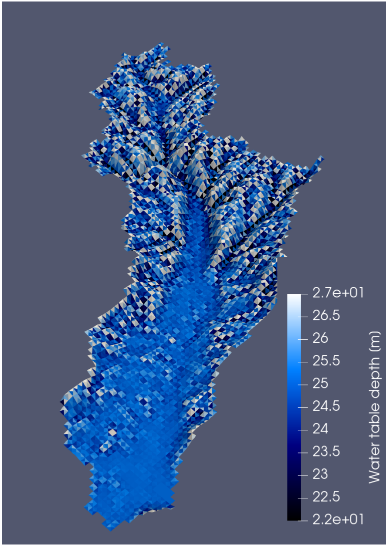


[1] Contributed to PETSc

TDycore preliminary application

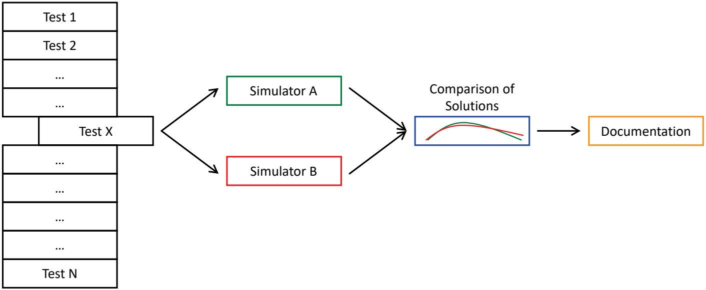
- South Fork Shoshone watershed, WY
- HUC8 watershed with 1685 km^2
- Grid cells: 436,320
- Water table initialized spatially homogeneously at a depth of 25m below to surface
- No flow boundary condition is applied

Water table depth after 30 days



Verification & Validation framework

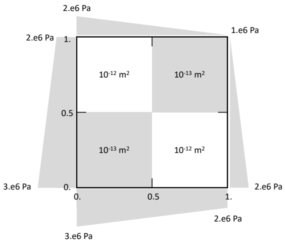
Developed an automated, python-based framework for V&V testing in the cloud that is code-agnostic

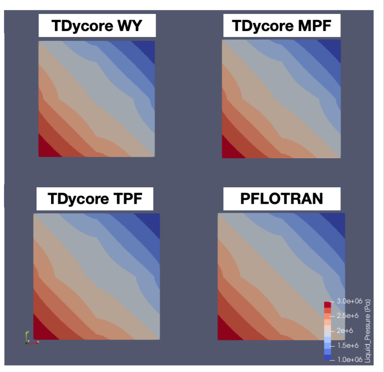


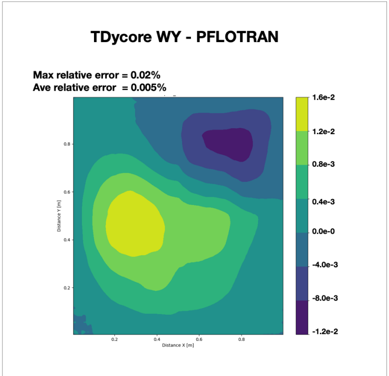
- The object-oriented framework compiles a list of tests to be run by a subset of simulators
- Results are compared among simulators, analytical solutions or empirical datasets
- Documentation is generated in reStructuredText format and compiled to pdf or html using Sphinx

Verification & Validation framework

- Steady-state, 2D saturated flow w/linear pressure gradient BCs and non-uniform block permeability.

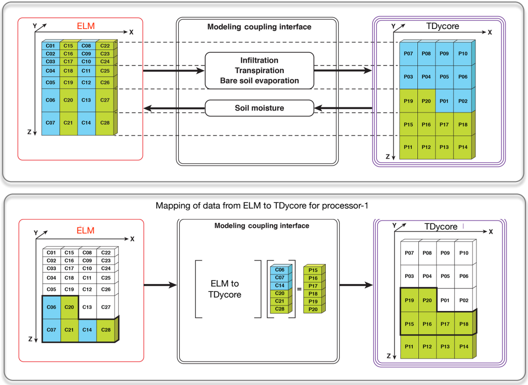






TDycore-ELM

- TDycore coupled to ELM through the **E**xternal **M**odel **I**nterface
- For mapping data between ELM and TDycore, a file format similar to the one use by coupler mapping files is used



Source: Modified from Bisht et al. (2017)

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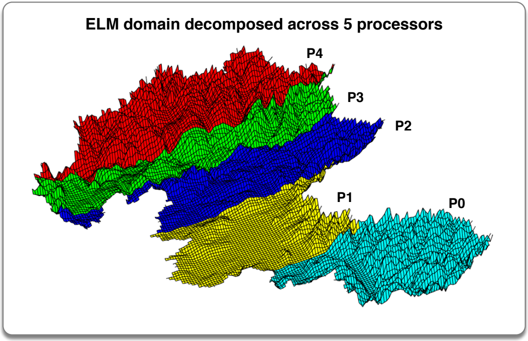
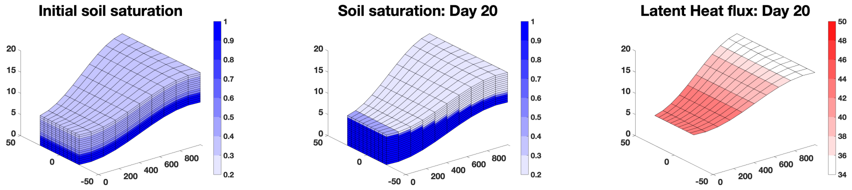
- ParMETIS to partition ELM during the run
- ELM mesh connectivity information is based on MPAS-O format



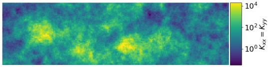
TDycore-ELM: Idealized simulation

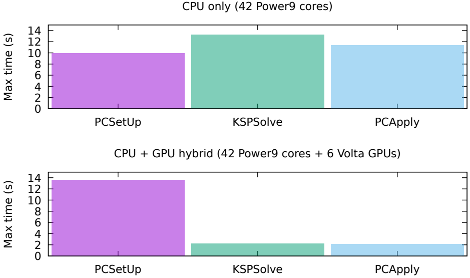
- A month long simulation with ELM-TDycore is performed for an idealized converging hillslope
  - Terrain-following initial soil moisture redistributes laterally
  - Higher soil moisture at the bottom of the hillslope leads to higher latent heat flux



SPE10 problem: Solver performance on Summit GPUs

SPE10: Permeability





- SPE10 problem performance on a node of OLCF Summit using GAMG with Chebyshev + Jacobi smoother.
- **5.9X speedup** observed in KSPSolve() when utilizing the Volta GPUs.
- Can utilize GPUs in PETSc solvers by specifying appropriate types on command line:

```
jsrun -n 6 -a 7 -c 7 -g 1 ./steady -dim 3 -N 200 -tdy_method wy -ksp_type cg
     -pc_type gamg -mg_levels_pc_type jacobi -dm_preallocate_only
     -dm_vec_type cuda -dm_mat_type aijcusparse
```

Thank you