Progress towards Continental-Scale Studies of Subsurface Hydrologic Processes in the United States using PFLOTRAN and CLM

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Abstract

Numerous studies have shown a positive soil moisture-rainfall feedback through observational data, as well as, modeling studies. Spatial variability of topography, soils, and vegetation play a significant role in determining the response of land surface states (soil moisture) and fluxes (runoff, evapotranspirtiaon); but their explicit accounting within Land Surface Models (LSMs) is computationally expensive. Additionally, anthropogenic climate change is altering the hydrologic cycle at global and regional scales. Characterizing the sensitivity of groundwater recharge is critical for understanding the effects of climate change on water resources. In order to explicitly represent lateral redistribution of soil moisture and unified treatment of the unsaturated-saturated zone in the subsurface within the CLM, we propose coupling PFLOTRAN and CLM.

In this work we present preliminary results obtained from the PFLOTRAN-CLM over a single soil column. Before preceding with the coupled model simulations over the entire globe, we propose to investigate the impact of improved representation of subsurface processes through a PFLOTRAN alone simulation over the Continental United States (CONUS), forced with CLM outputs.

PFLOTRAN: Massively Parallel Reactive Flow and Transport Code

- PFLOTRAN is a multiphase flow and multicomponent geochemical transport simulator currently under development as part of the DOE SciDAC-2 Program.
- Key PFLOTRAN features/capabilities either implemented or currently being implemented(*) include:
  - Object-oriented data structures
  - PETSc solvers and preconditioners
  - Modular linkage to physicochemical processes
  - Adaptive mesh refinement (AMR) based on SAMRAI
  - Unstructured Grids*
  - Multicontinuum subgrid model*
  - Multiphase flow, Non-isothermal transport
  - Multicomponent reactive transport
  - Biogeochemistry
  - Equilibrium and multirate sorption models
  - Surface complexation and ion exchange
  - Colloid-facilitated transport with mechanistic surface complexation model

PFLOTRAN: Unstructured mesh example

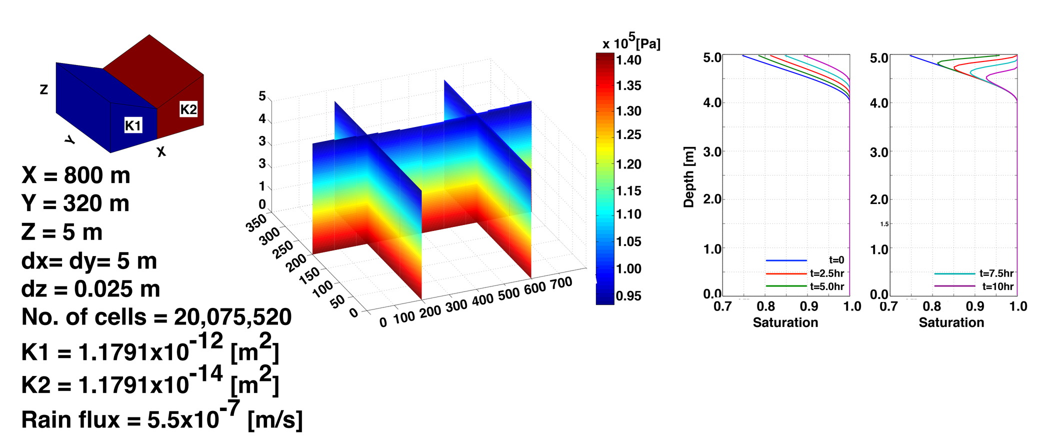
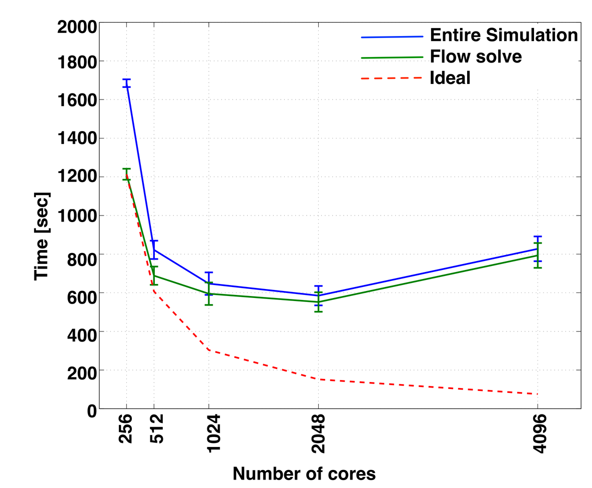


Figure 1: *V-Channel problem simulated by PFLOTRAN*



# of cores	Max. # of cells per core	Min. # of cells per core	Aveg. # of cells per core
256	81728	58110	78420
512	40646	26564	39210
1024	20368	12892	19605
2048	10190	2567	9802
4096	5078	2154	4901

Figure 2: *Performance of PFLOTRAN for a 20-million cell V-Channel problem*

Model formulations

CLM	PFLOTRAN
$\frac{\partial}{\partial t}(\theta) = -\nabla \cdot (\boldsymbol{q}) + q_w$	$\frac{\partial}{\partial t}(\rho\phi s) = -\nabla \cdot (\rho\boldsymbol{u}) + Q_w$
$\boldsymbol{q} = -K(\theta)\nabla(\psi + z)$	$\boldsymbol{u} = -\left(\frac{\kappa\kappa_r(s)}{\mu}\right)\nabla(P + \rho g z)$
$\psi = \psi_{sat}\left(\frac{\theta}{\theta_{sat}}\right)^{-B}$	$\psi = \frac{1}{\alpha}\left(\frac{s-s_r}{1-s_r}\right)^{-1/\lambda}$
$K(\theta) = K_{sat}\left(\frac{\theta}{\theta_{sat}}\right)^{3+2B}$	$\kappa(s) = \left(\frac{s-s_r}{1-s_r}\right)^{3+2/\lambda}$

$$\theta = \phi s \qquad K = \frac{\rho g \kappa}{\mu} \qquad P = \rho g \psi$$

θ - Soil moisture; ϕ - Soil porosity; s - Soil saturation
K - Hydraulic conductivity; κ - Permeability; ρ - Density of water
P - Pressure head; ψ - Matric potential

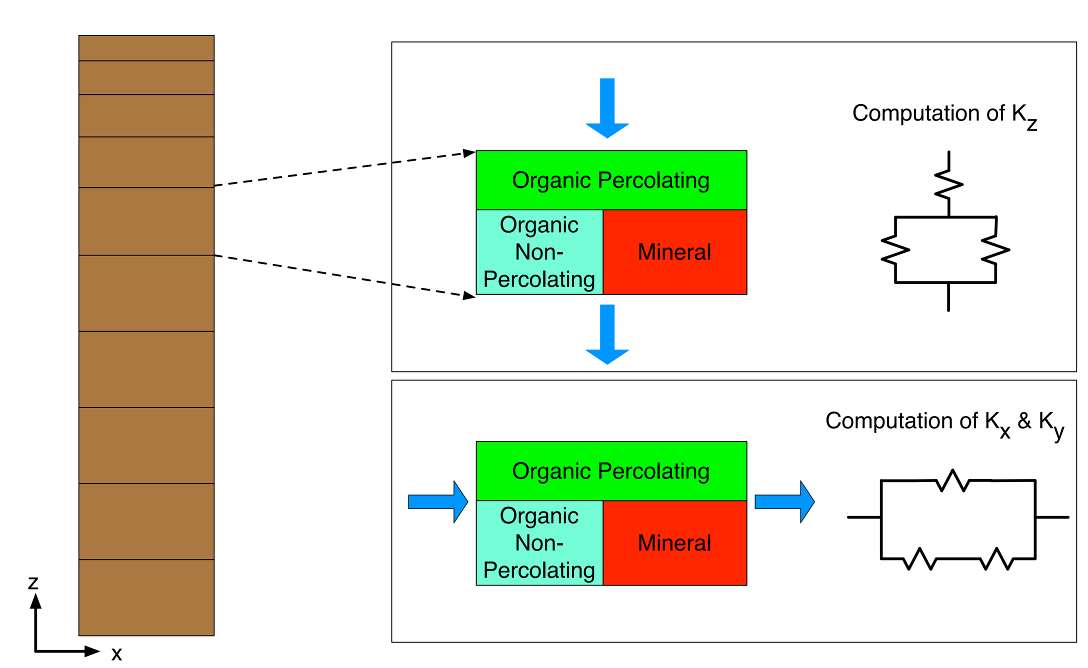


Figure 3: *Schematic representation of organic and mineral fraction within CLM soil layers*

PFLOTRAN-CLM coupled simulation over a single soil column

Experiment setup similar to Maxwell and Miller (2005, J. of HydroMeterology)

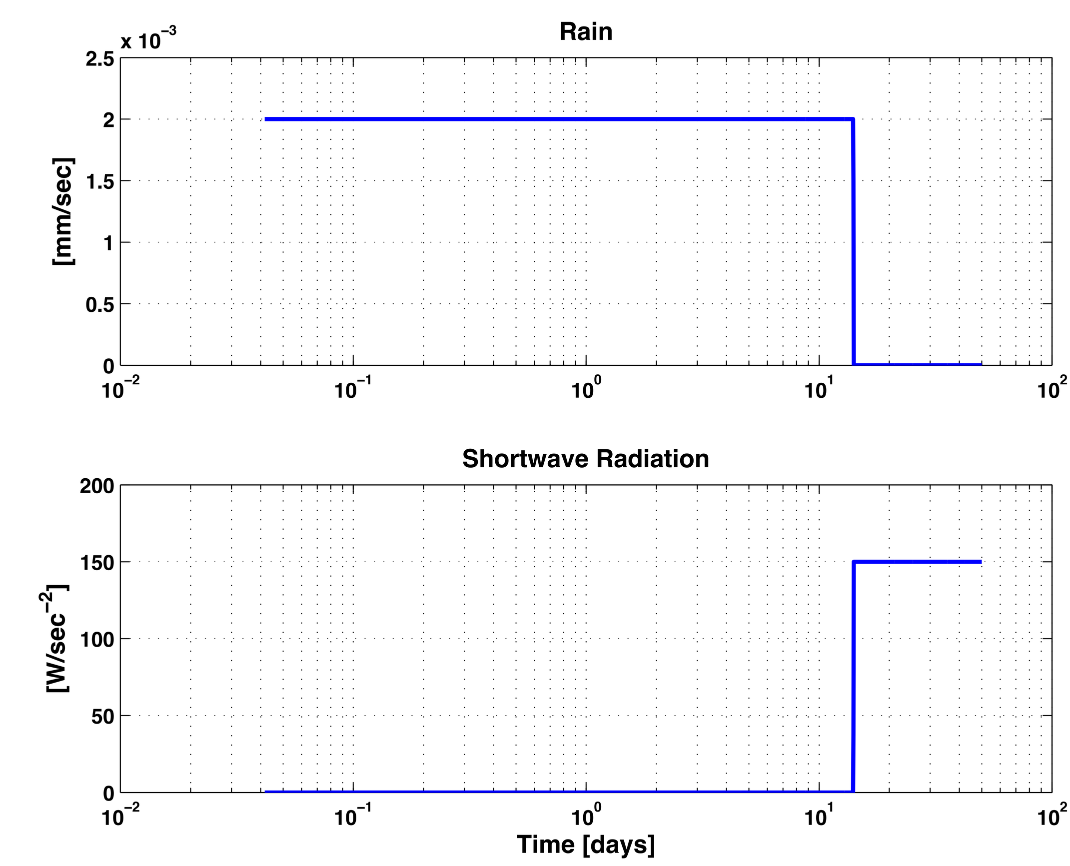


Figure 4: *Time series of rainfall and shortwave radiation forcings*

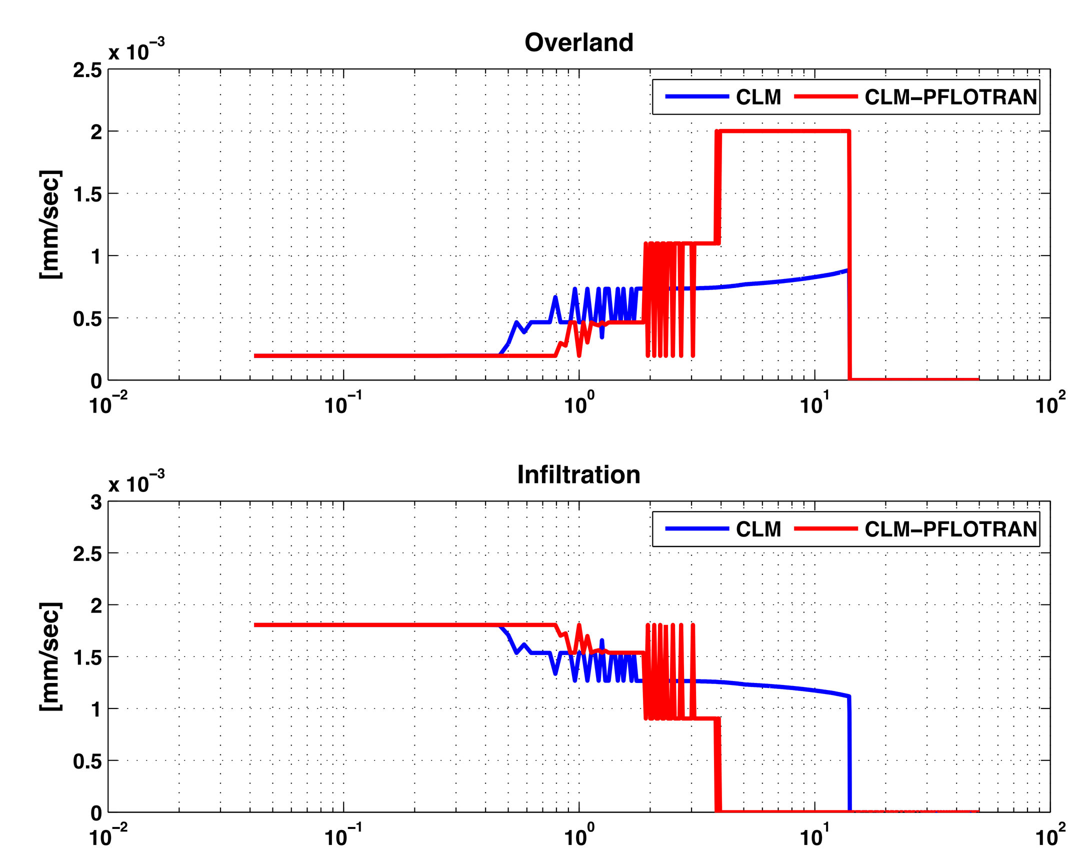


Figure 5: *Time series of simulated overland flow and infiltration by CLM and CLM-PFLOTRAN*

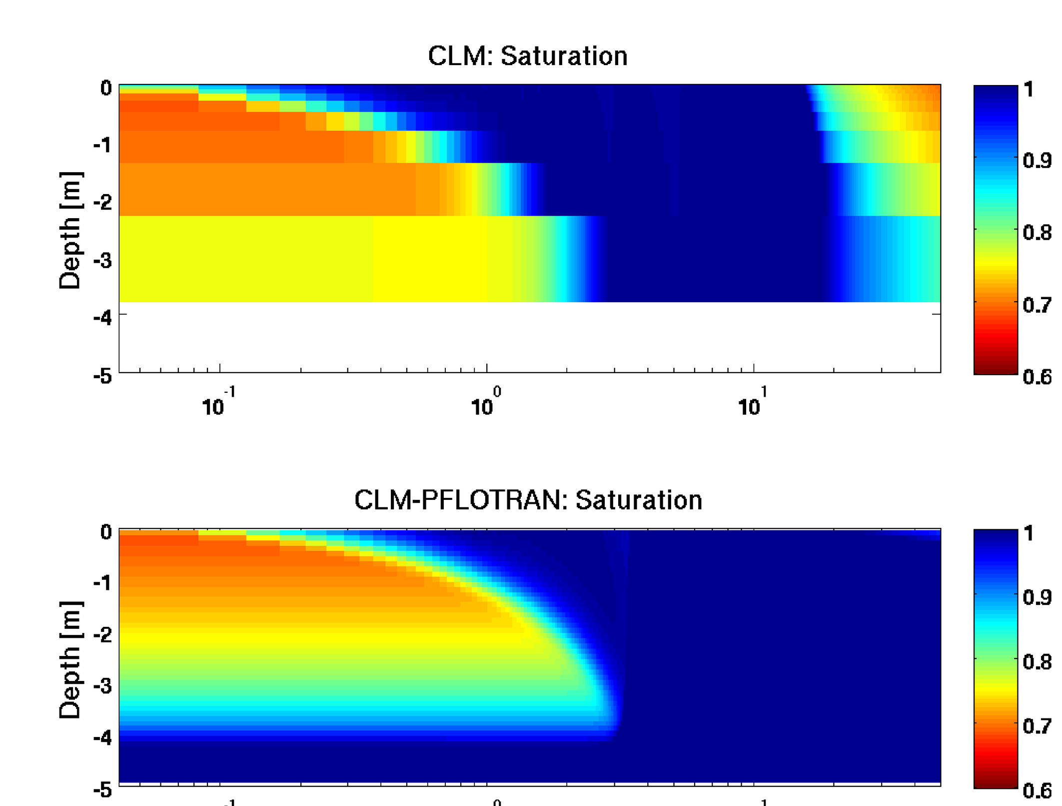


Figure 6: *Time series of simulated soil saturation by CLM and CLM-PFLOTRAN*

Model domain over the Continental United States

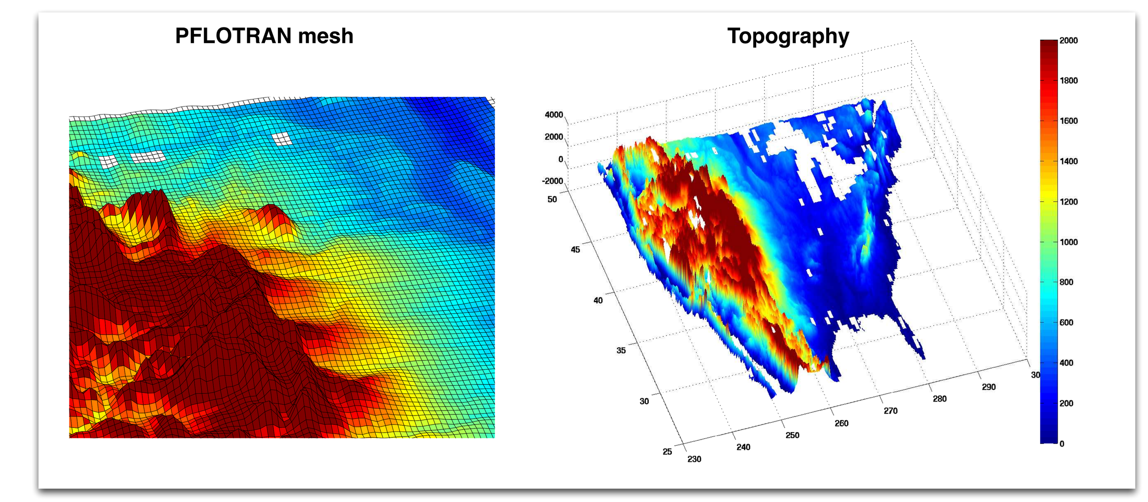


Figure 7: *Unstructured mesh of PFLOTRAN and topography for CONUS*

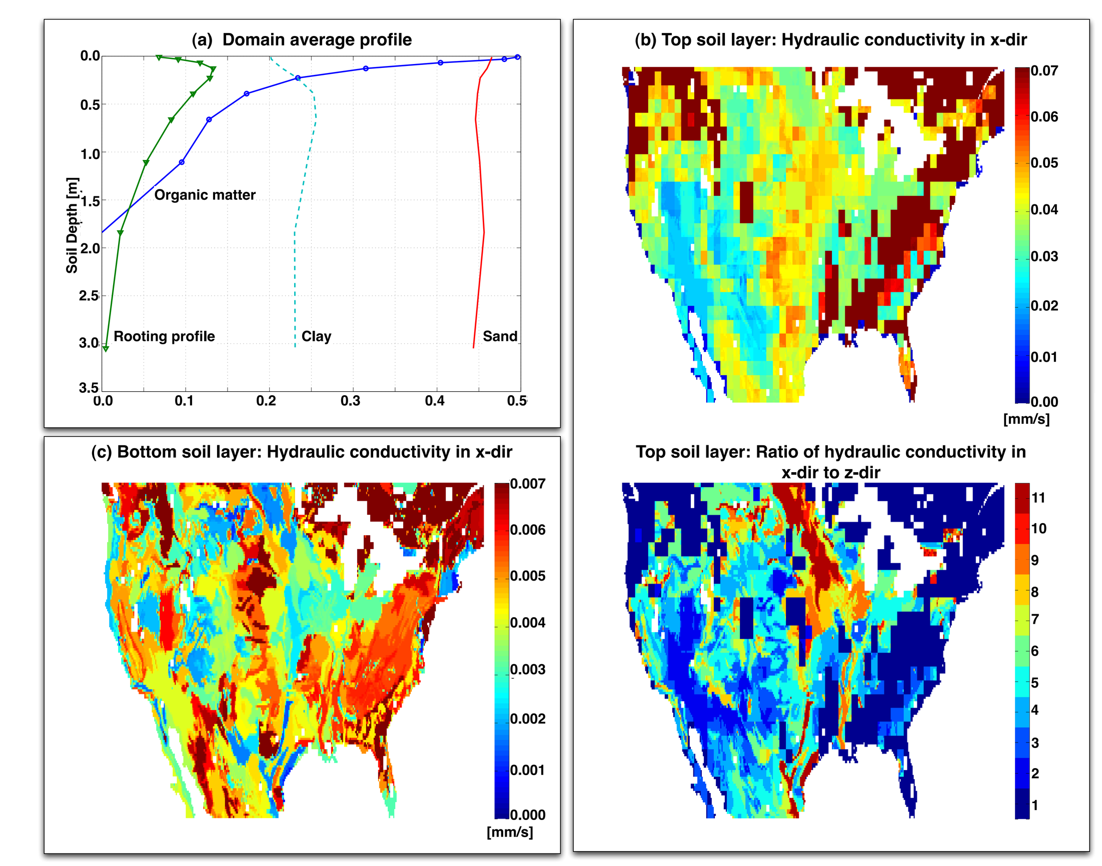


Figure 8: *(a) Domain average vertical profiles of organic matter, rooting profile, sand, and clay for CONUS domain. (b) Top layer hydraulic conductivity and anisotropy ratio. (c) Bottom layer hydraulic conductivity.*

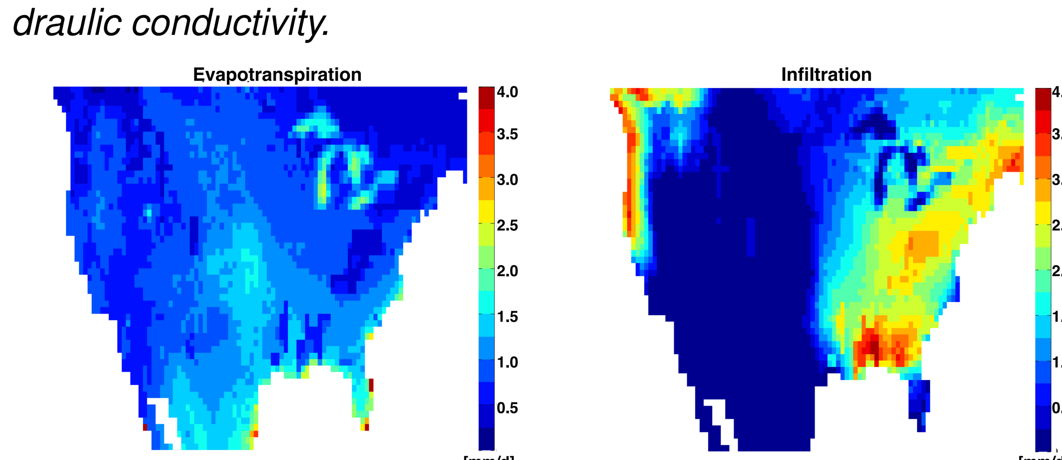


Figure 9: *Annual average evapotranspiration and infiltration simulated by CLM*

Future Directions

- Investigate the impact of incorporating lateral transport of soil moisture by performing offline PFLOTRAN simulation driven with CLM forcings.
- Study the feedback of lateral transport of soil moisture on surface processes by performing coupled PFLOTRAN-CLM simulations.

Acknowledgment

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