Use of composable solvers to represent multiphysics hydrologic and thermal processes in CLM

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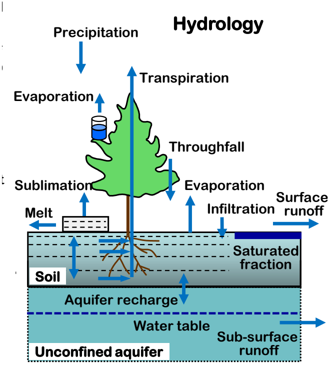
2015 LAND MODEL WORKING GROUP MEETING

Representation of subsurface hydrologic processes in CLM

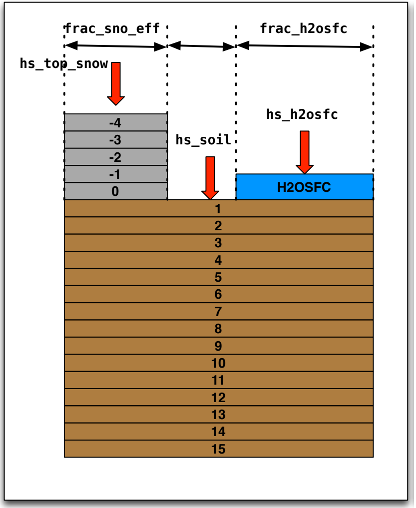
- θ-based Richards equation which is sequentially coupled to unconfined aquifer model.
- Spatial discretization: Finite Volume with 10 soil layers.
- Temporal discretization: Crank-Nicholson method.



Lawrence et al. (2011)

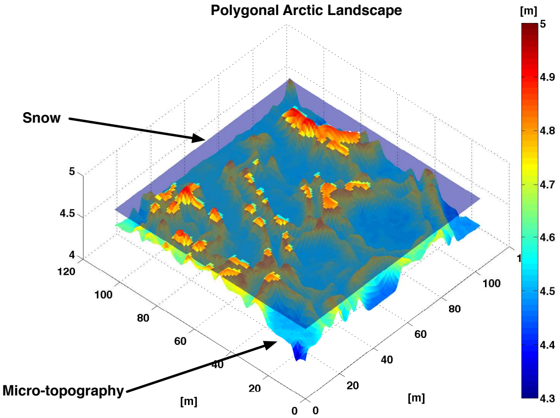
Representation of thermal processes in CLM

- Spatial discretization: Finite Volume with:
  - 5 (max) snow layers,
  - Surface water, and
  - 15 soil layers.
- Temporal discretization: Crank-Nicholson method.
- Phase change is accounted for the model.



Shortcomings of existing process representations in CLM

- Loosely coupled unsaturated-saturated subsurface hydrology.
- Extension of current formulations to include new processes is not straight forward.
- Few examples of new processes in this work include:
  - Macropore flow,
  - Lateral heat transport due to heterogeneous snow depth.



Portable, Extensible Toolkit for Scientific Computation

- The new modeling framework uses PETSc.
- Developed at Argonne National Laboratory.
- "*PETSc is a suite of data structures and routines for the scalable (parallel) solution of scientific applications modeled by partial differential equations*"[1]
- Provides solution to following types of problems:
  - Linear equation: $Ax = b$
  - Nonlinear equation: $F(x) = 0$
  - Timestepping of ODE and DAE: $F(t, u, \dot{u}) = G(t, u)$

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    - `SoilWaterMovementMod()`
    - `LakeTemperatureMod()`
    - `SoilTemperatureMod()`
  - Nonlinear equation: $F(x) = 0$
    - `CanopyFluxesMod()`
    - `CanopyTemperatureMod()`
  - Timestepping of ODE and DAE: $F(t, u, \dot{u}) = G(t, u)$

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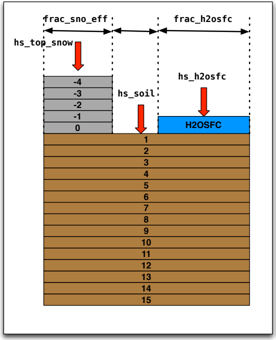
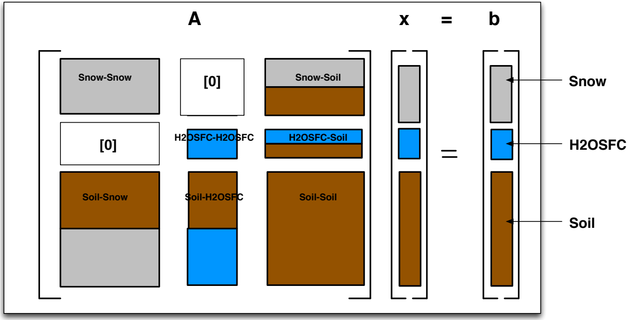
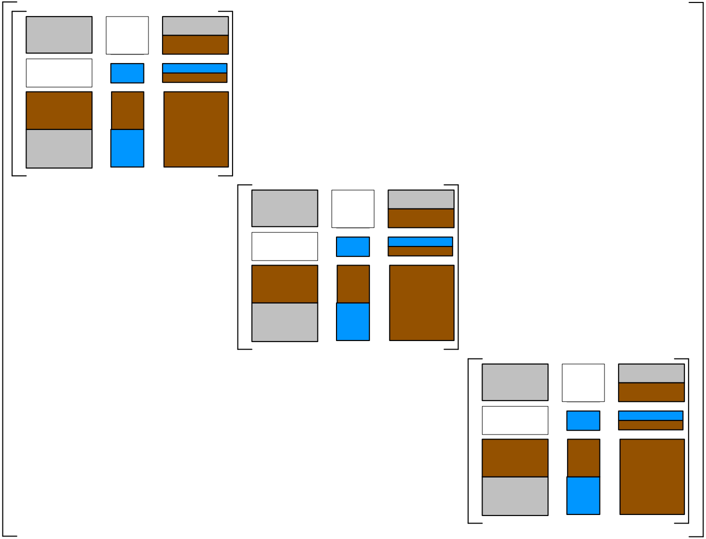
Example of a coupled “multiphysics” problem





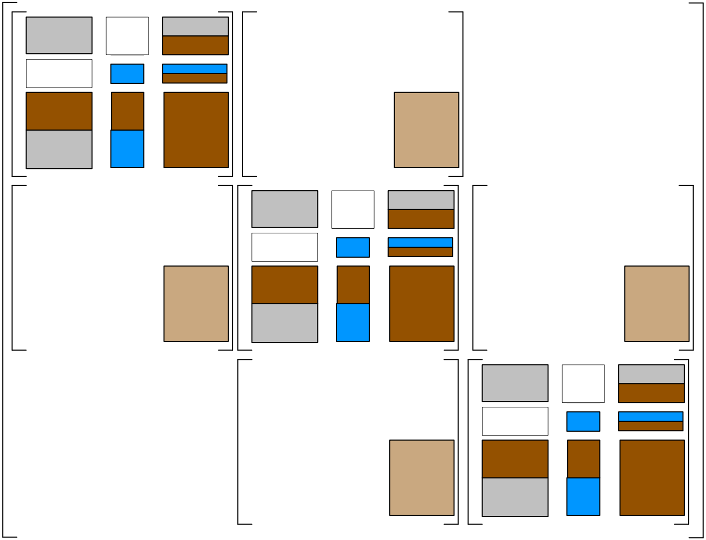
Example of a coupled "multiphysics" problem (cont'd)

- Matrix A for multiple columns that are independent.



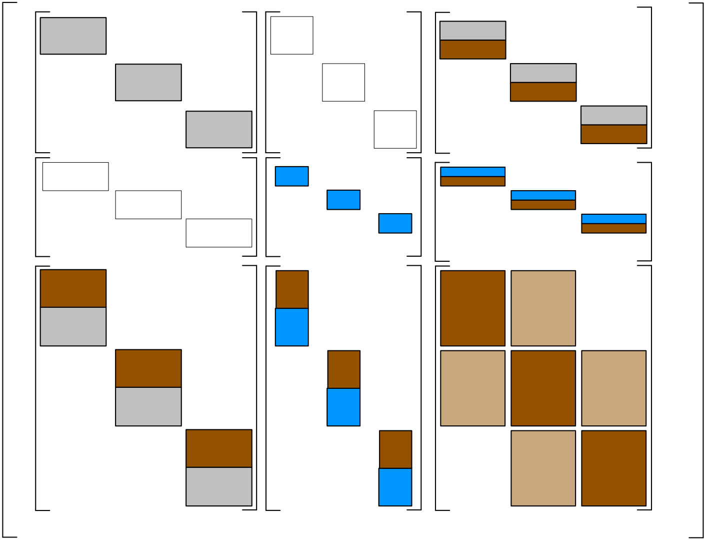
Example of a coupled "multiphysics" problem (cont'd)

- Matrix A for multiple columns with laterally connected soils.



Example of a coupled “multiphysics” problem (cont’d)

- PETSc representation of Matrix A.



Example of a coupled "multiphysics" problem (cont'd)

```
subroutine AssembleMatrix(A)

 ! Get diagonal matrices
 call MatGetSubmatrix(A,0,0,A_snow)
 call MatGetSubmatrix(A,1,1,A_sfc)
 call MatGetSubmatrix(A,2,2,A_soil)

 ! Get off-diagonal matrices
 call MatGetSubmatrix(A,0,2,A_snow_soil)
 call MatGetSubmatrix(A,1,2,A_sfc_soil)
 call MatGetSubmatrix(A,2,0,A_soil_snow)
 call MatGetSubmatrix(A,2,1,A_soil_sfc)
```

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 call MatGetSubmatrix(A,1,2,A_sfc_soil)
 call MatGetSubmatrix(A,2,0,A_soil_snow)
 call MatGetSubmatrix(A,2,1,A_soil_sfc)

 call AssembleMatSnow(A_snow)
 call AssembleMatSrfw(A_sfc)
 call AssembleMatSoil(A_soil)

 call AssembleMatSnowSoil(A_snow_soil)
 !Do the remaining steps
```

Variably Saturated Flow Model (VSFM)

Governing equations for flow in porous media are given by:

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

$$\mathbf{q} = -\frac{k k_r}{\mu} \nabla (P + \rho g z) \tag{2}$$

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Approach-1: Use PETSc non-linear solver (PFLOTRAN formulation)

$$\frac{(\phi s_w \rho)_i^{t+1} - (\phi s_w \rho)_i^t}{\Delta t} + \sum_j (\rho_{i,j} \mathbf{q}_{i,j})^{t+1} - S_i^{t+1} = 0 \tag{3}$$

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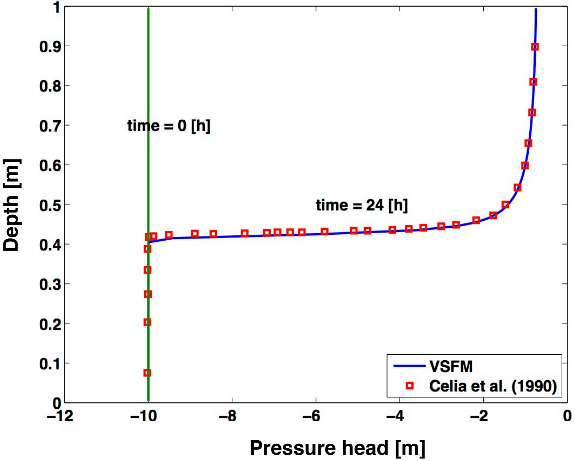
Approach-2: Use PETSc time stepper for DAE

$$\dot{\xi}_i - \sum_j (\rho_{i,j} \mathbf{q}_{i,j}) + S_i = 0 \tag{4}$$

$$\xi_i - (\phi s_w \rho)_i = 0 \tag{5}$$

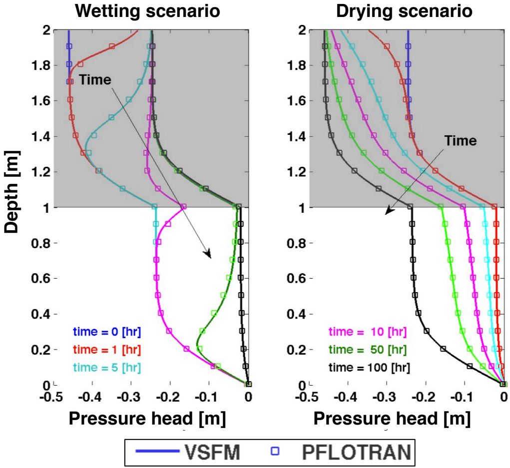
P-1: Infiltration in a very dry soil

- 1 [m] deep soil column (Celia et al. (1990)).
- Conditions
  - IC : $P(z, t = 0) = -10$[m]
  - BC: $P(z = 0, t) = -0.75$[m]
- Model captures the sharp wetting profile at $t = 24$ [hr].



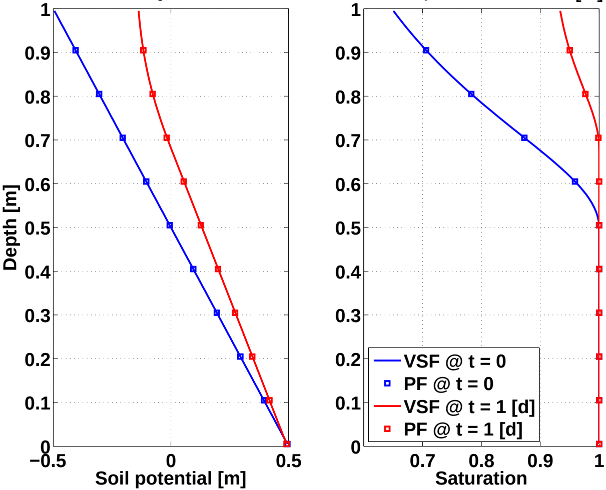
P-2: Transient flow in layered soils

- Evolution of pressure profile between two steady state conditions.
- $K_{s,top}/K_{s,bot} = 10$
- Top boundary conditions
  - Wetting flux: 2.5×10^{-6} [m s^{-1}]
  - Drying flux: 2.8×10^{-8} [m s^{-1}]



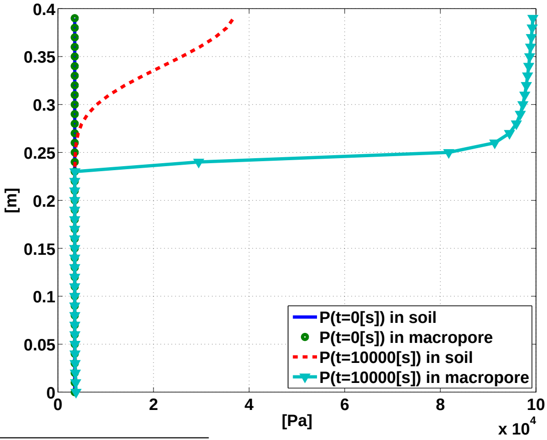
P-3: Water table dynamics

- Soils are same as in Celia et al. (1990).
- Conditions
  - IC : Hydrostatic condition with water table at 0.5 [m]
  - BC: Top flux $= 2.5 \times 10^{-5}$ [m s^{-1}]
- The simulated steady state water table depth at $t = 1$[d] is 0.7 [m].



P-4: Macropore flow

- Dual continuum connected matrix[2] problem described in Gerke and van Genuchten (1993)
- $V_{mpore} = 0.05 V_{total}$; $K_{mpore} \approx 2000 \times K_{soil}$
- Constant infiltration flux (50 [cm/d]) is applied only in the macropore.



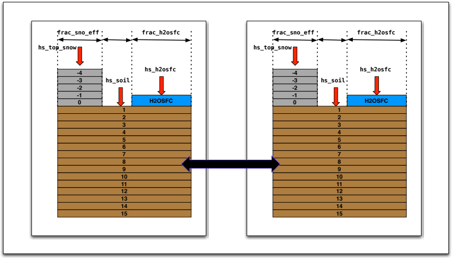
[2] Lichtner, P. C. (2000)

Lateral heat transport in the subsurface

Governing equations for heat conduction are given by:

$$c\frac{\partial T}{\partial t} = -\nabla \cdot (\mathbf{q}) + S \qquad (6)$$

$$\mathbf{q} = -\lambda \nabla (T) \qquad (7)$$

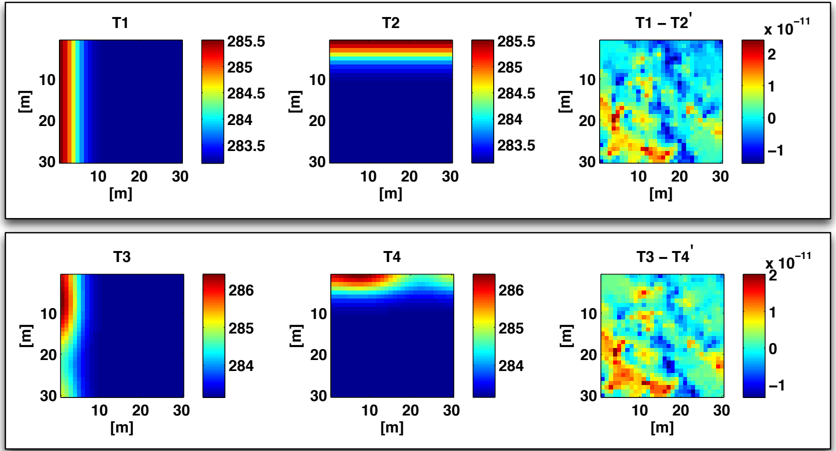


Use PETSc linear solver

$$\frac{c_i \Delta V_i}{\Delta t}(T_i^{t+1} - T_i^t) = -\alpha \sum_j (\mathbf{q}_{i,j})^{t+1} - (1-\alpha) \sum_j (\mathbf{q}_{i,j})^t + S_i^{t+1} \qquad (8)$$

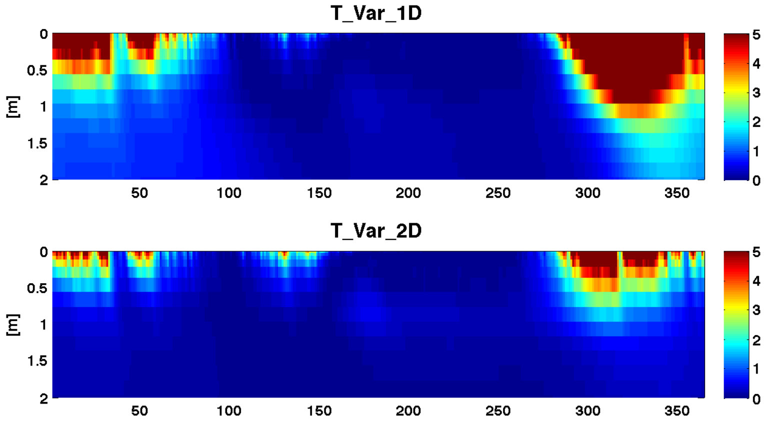
P-5: Propagation of temperature perturbation

- Evolution of an initial temperature perturbation applied to (i) top, and (ii) left control volumes studied.
- Two types of temperature perturbation are applied: (i) spatially homogenous; and (ii) sinusoidally varying.



P-6: Lateral thermal transport in Arctic polygonal ground

- Simulation for a transect in a polygonal Arctic landscape.
- Heterogeneous snow depth due to microtopography.
- Differences in $\sigma^2_{T_s}$ when thermal processes are represented as 1D or 2D.



Summary

- A new modeling framework to couple multiphysics processes in CLM is developed using PETSc.
- The framework has been applied to hydrologic and thermal processes in CLM.
- The framework allows for:
  - Addition of new processes (e.g. soil–macropore flow), and
  - Extension to multi-dimensional process representation (e.g. lateral heat transport).

Acknowledgement

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