R: Composable solvers for multiphysics problems in ALM

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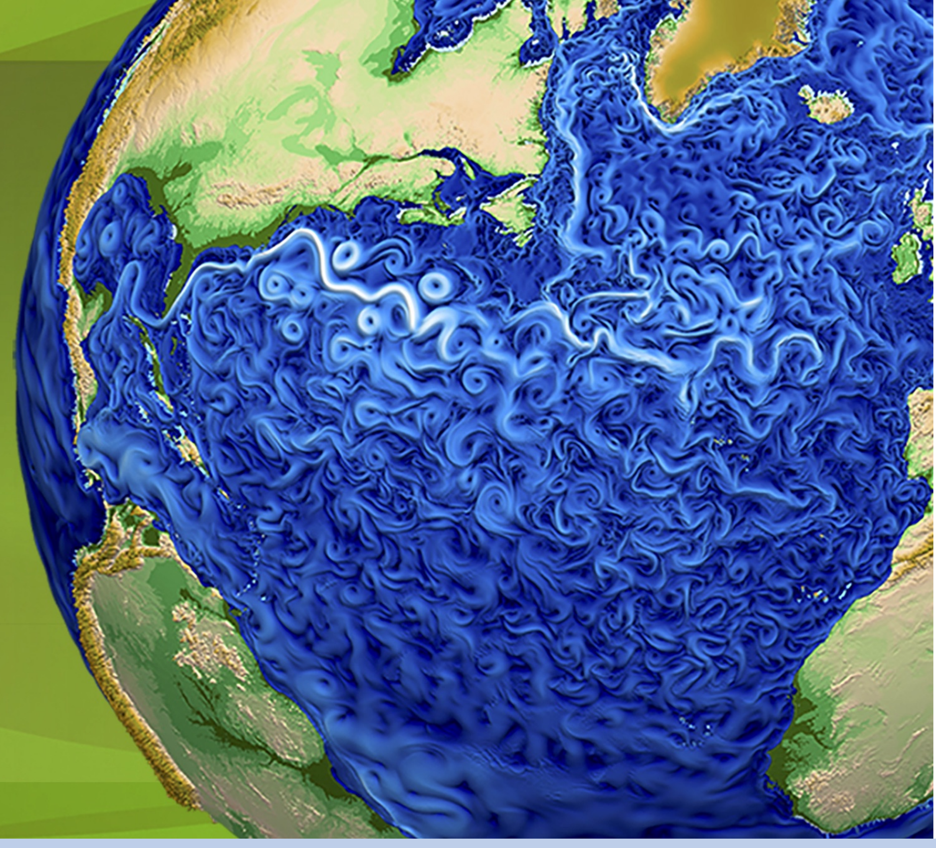


Objective

- Land surface models (LSMs), which are key components of Earth System Models (ESMs), simulate mass, energy, and nutrient cycles at the surface of the Earth.
- Traditionally, the various physics formulations in LSMs are solved as a loosely coupled system of equations.
- The importance of solving fully coupled multiphysics problems (e.g., soil-plant-atmosphere continuum, conservation of mass-energy in soil, etc.) is now well recognized.
- We present a framework for solving tightly coupled multi physics problems (MPP) using the Portable, Extensible Toolkit for Scientific Computation (PETSc).

Model

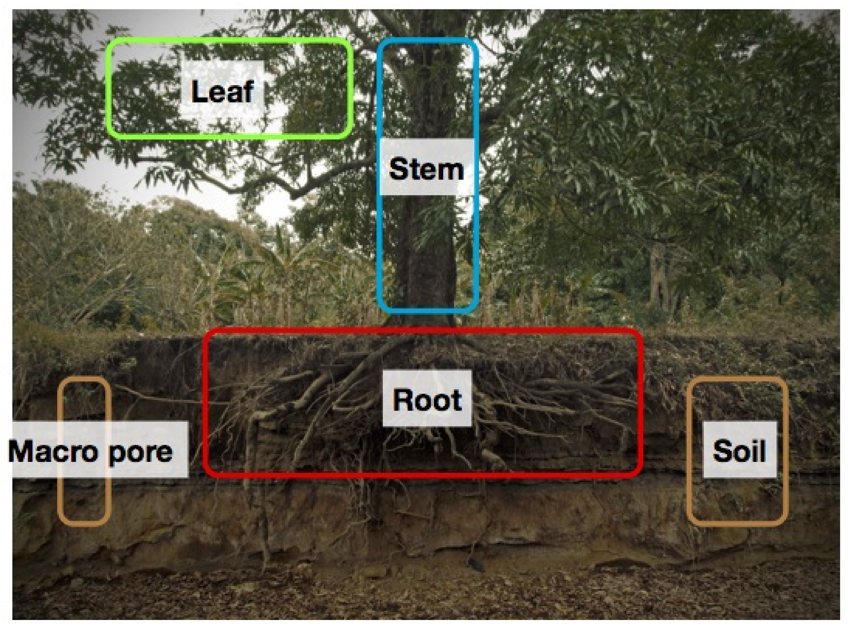
The governing equations for mass and energy are given by

$$\frac{\partial(\rho s\phi)}{\partial t} = -\nabla\cdot(\rho\vec{q}) + Q_{water}$$

and

$$\frac{\partial}{\partial t}(\rho s\phi U + (1-\phi)\rho_{soil}C_{soil}T) = -\nabla\cdot(\rho\vec{q}H - \kappa\nabla T) + Q_{energy}$$

- MPP framework accommodates definition of separate equations for the various comments.
- In case of a nonlinear system of equations, the MPP framework computes for each equation:
  - Residual,
  - Diagonal Jacobian block, and
  - Off-digonal Jacobian block.
- PETSc DMComposite() is used to assemble and solve the tightly coupled system of discretized equations.

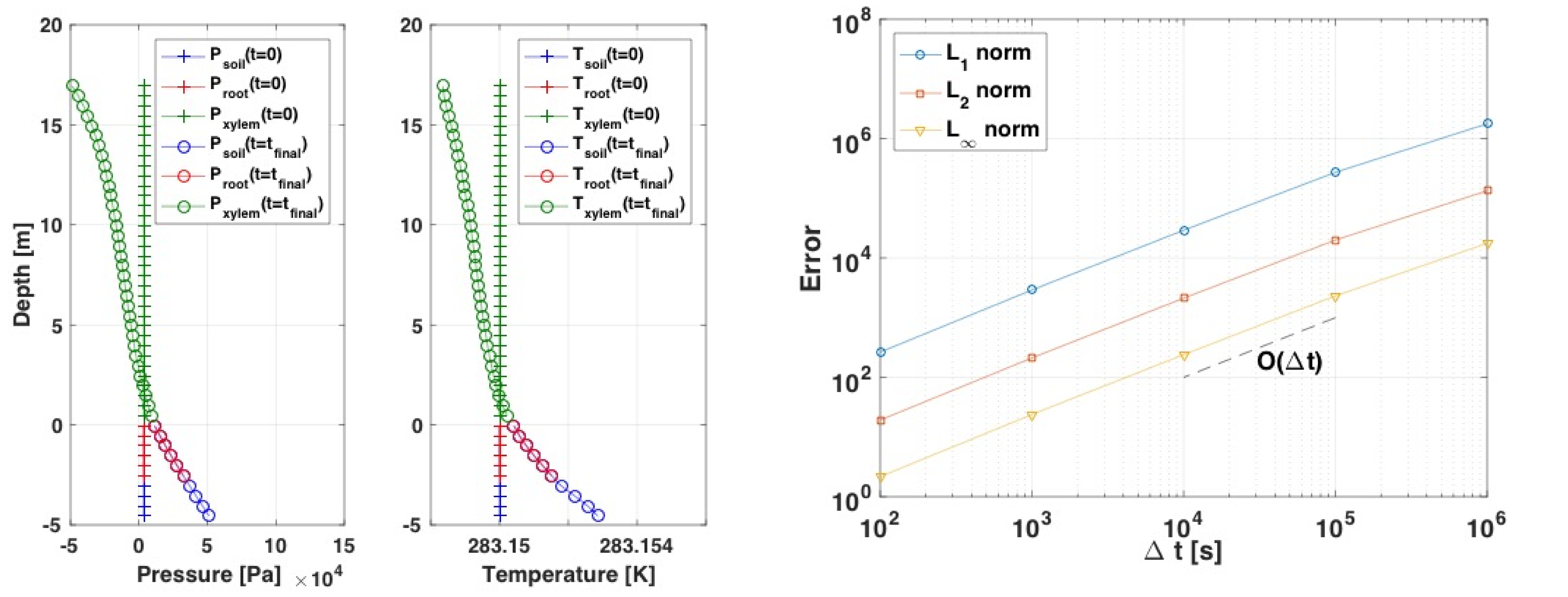


Schematic representation of numerical solution via Newton's method for mass and energy equation in soil-root-xylem system is given by:

$$\begin{pmatrix}
\left[\frac{\partial R_s^{mass}}{\partial P_s}\right] & \left[\frac{\partial R_s^{mass}}{\partial P_r}\right] & [0] & \left[\frac{\partial R_s^{mass}}{\partial T_s}\right] & \left[\frac{\partial R_s^{mass}}{\partial T_r}\right] & [0] \\
\left[\frac{\partial R_r^{mass}}{\partial P_s}\right] & \left[\frac{\partial R_r^{mass}}{\partial P_r}\right] & \left[\frac{\partial R_r^{mass}}{\partial P_x}\right] & \left[\frac{\partial R_r^{mass}}{\partial T_s}\right] & \left[\frac{\partial R_r^{mass}}{\partial T_r}\right] & \left[\frac{\partial R_r^{mass}}{\partial T_x}\right] \\
[0] & \left[\frac{\partial R_x^{mass}}{\partial P_r}\right] & \left[\frac{\partial R_x^{mass}}{\partial P_x}\right] & [0] & \left[\frac{\partial R_x^{mass}}{\partial T_r}\right] & \left[\frac{\partial R_x^{mass}}{\partial T_x}\right] \\
\left[\frac{\partial R_s^{energy}}{\partial P_s}\right] & \left[\frac{\partial R_s^{energy}}{\partial P_r}\right] & [0] & \left[\frac{\partial R_s^{energy}}{\partial T_s}\right] & \left[\frac{\partial R_s^{energy}}{\partial T_r}\right] & [0] \\
\left[\frac{\partial R_r^{energy}}{\partial P_s}\right] & \left[\frac{\partial R_r^{energy}}{\partial P_r}\right] & \left[\frac{\partial R_r^{energy}}{\partial P_x}\right] & \left[\frac{\partial R_r^{energy}}{\partial T_s}\right] & \left[\frac{\partial R_r^{energy}}{\partial T_r}\right] & \left[\frac{\partial R_r^{energy}}{\partial T_x}\right] \\
[0] & \left[\frac{\partial R_x^{energy}}{\partial P_r}\right] & \left[\frac{\partial R_x^{energy}}{\partial P_x}\right] & [0] & \left[\frac{\partial R_x^{energy}}{\partial T_r}\right] & \left[\frac{\partial R_x^{energy}}{\partial T_x}\right]
\end{pmatrix}
\begin{pmatrix}
[\Delta P_s^{mass}] \\ [\Delta P_r^{mass}] \\ [\Delta P_x^{mass}] \\ [\Delta T_s^{energy}] \\ [\Delta T_r^{energy}] \\ [\Delta T_x^{energy}]
\end{pmatrix}
= -
\begin{pmatrix}
[R_s^{mass}] \\ [R_r^{mass}] \\ [R_x^{mass}] \\ [R_s^{energy}] \\ [R_r^{energy}] \\ [R_x^{energy}]
\end{pmatrix}$$

Result : Soil–Root–Xylem

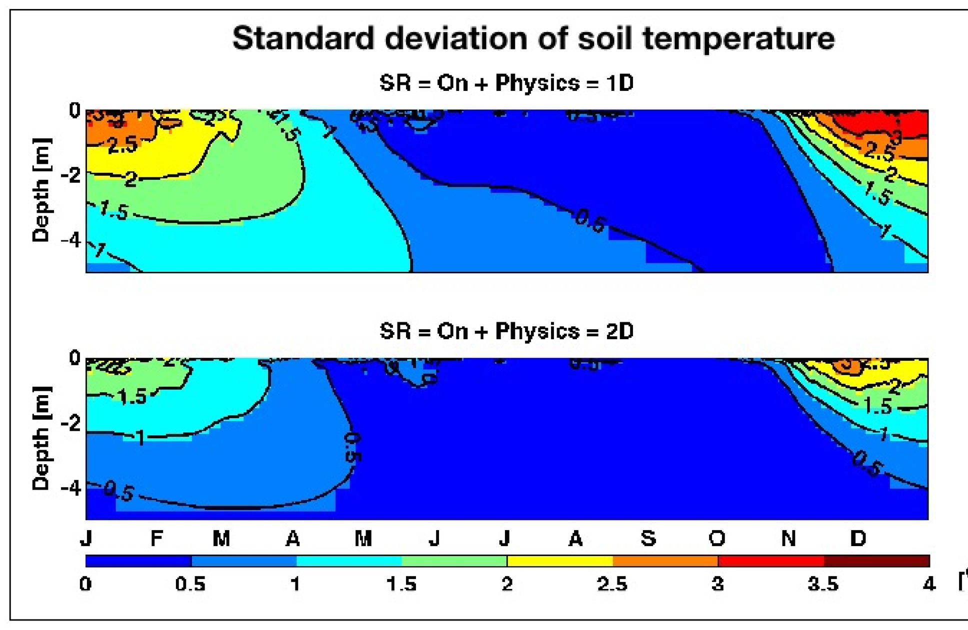
- Soil domain: 1x1x5 [m] ; Root domain: 1x1x3 [m]; Xylem domain: 1x1x17 [m].
- Initial condition: Constant pressure and constant temperature.
- No flow boundary conditions and the simulation duration is 10^6 [s].
- Soil pressure redistributes vertically towards a hydrostatic condition with negligible change in temperature.
- Validation of the backward Euler integration scheme is obtained by the linear convergence of the L_1, L_2 and L_∞ error of the numerical solution.

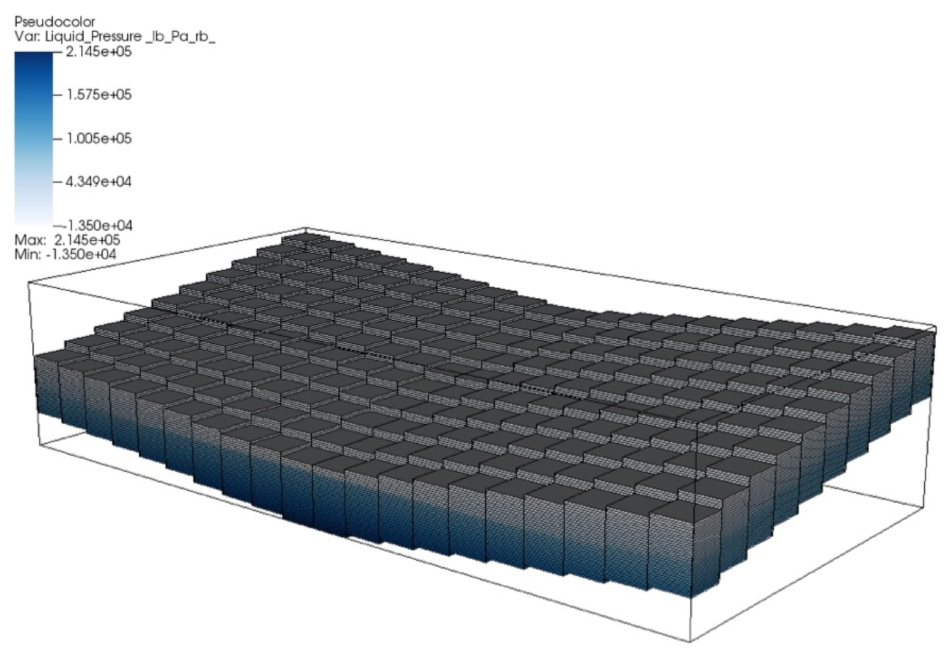


Moving beyond 1-Dimensional model

The multiphysics framework supports mutlidimensional problems.

- Microtopographic features in Arctic lead to heterogeneous snow depth.
- Accounting for snow redistribution (SR) results in surface T_{soil} heterogeneity that propagates deeper in the soil column.
- 1D subsurface thermal model overestimates $\sigma_{T_{soil}}$ when compared to 2D physics formulation.





- Option to decompose ALM grid using ParMETIS has been added.
- Lateral flow models of various complexity are being explored:
  - Modified 1D with lateral flow as source/sink,
  - Operator split approach: 1D + 2D, or
  - Full 3D

ACME Accelerated Climate Modeling for Energy

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