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

\[
\frac{\partial (\rho \phi)}{\partial t} = -\nabla \cdot (\rho \mathbf{q}) + Q_{\text{water}}
\]

and

\[
\frac{\partial (\rho \mathbf{U} + (1 - \phi) \rho_{\text{soil}} C_{\text{soil}} T)}{\partial t} = -\nabla \cdot (\rho \mathbf{q} H - \kappa \nabla T) + Q_{\text{energy}}
\]

- 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:

\[
\begin{bmatrix}
\left[ \frac{\partial \phi}{\partial x} \right] & \left[ \frac{\partial \phi}{\partial y} \right] & \left[ 0 \right] & \left[ 0 \right] & \left[ \Delta \phi \right]
\end{bmatrix}^T =
\begin{bmatrix}
\left[ R_{\phi} \right] \\
\left[ R_{\phi} \right] \\
\left[ R_{\phi} \right] \\
\left[ R_{\phi} \right] \\
\left[ 0 \right]
\end{bmatrix}
\]

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 $10^8$ [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 $L_\infty$ error of the numerical solution.

Moving beyond 1-Dimensional model

The multiphysics framework supports multidimensional problems.

- Microtopographic features in Arctic lead to heterogeneous snow depth.
- Accounting for snow redistribution (SR) results in surface $T_{\text{soil}}$ 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