Multi-Physics Problem library for terrestrial biophysics processes: Initial development & applications

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Motivation: Scientific requirements

- Current generation land surface models (LSMs), including ELM, routinely neglect many critical multi-component, multi-physics processes including:
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  - How hydraulic functional traits of root, stem, and leaf will determine the response of trees to future drought?

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  - **Lateral redistribution of soil moisture**
    - How topography may mitigate drought effects on vegetation along a hillslope gradient?

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Tai et al. (2017) New Phytologist
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  - **Lateral redistribution of soil moisture**
    - How topography may mitigate drought effects on vegetation along a hillslope gradient?
  
  - **Adveective transport of energy**
    - Will inclusion of advective energy transport significantly alter prediction of permafrost thaw?
Motivation: Computational requirements

- ELM’s existing **numerical algorithms are inadequate** for solving tightly coupled, multi-dimensional, multi-physics problems
- ELM’s **monolithic software design** is not extensible to support solution of tightly coupled multi-physics problems
- Numerical implementation of processes in ELM are coded for a **single spatial-temporal discretization** and a **fixed set of boundary and source-sink conditions**
Multi-Physics Problem (MPP) library

- Challenges of efficiently solving multi-physics problems are not unique to the LSM community
- Uses PETSc to provide numerical solution of discretized equations
- PETSc’s DMComposite is used to solve tightly coupled multi-physics problems
- Open source available at https://github.com/MPP-LSM/MPP
- Follows an open development framework
- Using Travis-CI for testing on Linux and OS X
- Solution verification is being performed via method of manufactured solutions
Outline

1. Application of MPP to solve subsurface hydrologic processes
   - Single physics, single component
2. Application of MPP to solve subsurface thermal processes with lateral redistribution of energy
   - Single physics, multi dimension
3. Application of MPP to resolve transport of water through soil-plant continuum
   - Single physics, multi component
4. Verification for MPP
Improving subsurface hydrologic processes in ELM

- Groundwater is a source for 30% of all freshwater withdrawals used for agriculture, domestic, and industrial purposes.
- ELM-v0 treats subsurface hydrologic processes separately in unsaturated and saturated zone.
- Water table observation of Fan et al. (2013) is deeper than the extent of soil ELM soil column for 13% of land grid cells.
**Variably Saturated Flow Model (VSFM)**

**Model:**
- A **unified physics formulation** is developed in ELM-v1 to solve subsurface hydrologic processes in a variably saturated soil.
- Spatial and temporal discretization leads to a set of nonlinear equations that are solved using PETSc.
- Global offline ELM simulations showed that subsurface drainage flux ($q_{\text{drain}}$) had a dominant control on predicted water table depth (WTD)

$$q_{\text{drain}} = q_{\text{drain, max}} \exp(-f_{\text{drain}} z_{\text{WTD}})$$
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\]

Simulation configuration:

- Vertical discretization of soil column was modified to include 59 soil layers that reached a depth of 150 m.

- An ensemble of global simulations with multiple \(f_{\text{drain}}\) values were performed for 200-years on \(1.9^\circ \times 2.5^\circ\) grid to estimate an optimal \(f_{\text{drain}}\) for each grid cell.

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Estimation of $f_{\text{drain}}$ parameter
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Bisht et al. (2018) GMDD, in review
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Simulated water table depth anomalies

<table>
<thead>
<tr>
<th>ELM with default $f_{\text{drain}}$</th>
<th>ELM with estimated $f_{\text{drain}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bias</td>
<td>RMSE</td>
</tr>
<tr>
<td>-10.3</td>
<td>21.3</td>
</tr>
</tbody>
</table>
Objective:
- How spatial heterogeneity of soil temperature due to spatially variable snow depth is impacted by inclusion of lateral redistribution of heat?

Model:
- Incorporated lateral energy transport in the subsurface within ELM.
- Spatial and temporal discretization leads to a set of linear equations that are solved via PETSc.

Simulation configuration:
- 10-years long simulations for a two-dimensional transect across polygonal landscape at the Barrow Environmental Observatory, AK are run for 1D and 2D physics formulation.
Simulated soil temperature profiles

The model accurately reproduces observed soil temperature vertical profiles in the polygon rims and centers

Bisht et al. (2017), GMD
The model **accurately reproduces observed soil temperature** vertical profiles in the polygon **rims** and **centers**.
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Bisht et al. (2017), GMD
Simulated soil temperature spatial variability

Timeseries of spatial standard deviation for each soil layer averaged

Excluding lateral subsurface thermal processes had modest impact on mean states (not shown here) but an overestimation of spatial variability in soil temperature

Bisht et al. (2017), GMD
Application of VSFM to resolve plant hydraulics

- VSFM uses PETSc's extensible framework (DMComposite) to resolve **tightly coupled** transport of water through the soil-plant continuum.
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Solution of nonlinear equations for a soil system

\[
(J_{s,s}) (\Delta X_s) = -(R_s)
\]
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Solution of nonlinear equations for a soil-root system

\[
\begin{pmatrix}
J_{s,s} & J_{s,r} \\
J_{r,s} & J_{r,r}
\end{pmatrix}
\begin{pmatrix}
\Delta X_s \\
\Delta X_r
\end{pmatrix}
= -
\begin{pmatrix}
R_s \\
R_r
\end{pmatrix}
\]
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Solution of nonlinear equations for a soil-root-xylem system

\[
\begin{pmatrix}
J_{s,s} & J_{s,r} & 0 \\
J_{r,s} & J_{r,r} & J_{r,x} \\
0 & J_{x,r} & J_{x,x}
\end{pmatrix}
\begin{pmatrix}
\Delta X_s \\
\Delta X_r \\
\Delta X_x
\end{pmatrix}
= -
\begin{pmatrix}
R_s \\
R_r \\
R_x
\end{pmatrix}
\]
Application of VSFM to resolve plant hydraulics

- Collaborating with Gil Bohrer and Golnazalsadat Mirfenderesgi (OSU), developers of FETCH2
- Study site: US-UMB contains Oak and Pine; Study period: 2015-2017
- Vertical profile of potential transpiration is derived based on meteorological data and tree characteristics
- Model computes vertical transport of water and actual transpiration based on leaf water potential
Verification via Method of Manufactured Solutions (MMS)

- Validation: Solving the correct equations?
- Verification: Solving the equations correctly?
- MMS is an approach used for model verification
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**Model:**
\[
0 = -\nabla \cdot (-\lambda \nabla T) + Q
\]

**Manufacture a solution:**
\[
T(x, y, z) = 10 \sin(x\pi) \cos(2y\pi) \sin(3z\pi) + 270
\]
\[
\lambda(x, y, z) = \exp(x + y + z - 1)
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Derive \( Q(x, y, z) \) by substituting the manufactured solution into the model.
Prescribe \( Q \) to each grid cell in the numerical model and solve for \( T(x, y, z) \).
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Thank you