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

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April 12, 2018

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Manoli et al. (2017), Adv. Water Res.

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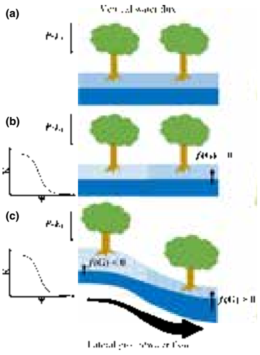
- Lateral redistribution of soil moisture
  - How topography may mitigate drought effects on vegetation along a hillslope gradient?



Tai et al. (2017) New Phytologist

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- Lateral redistribution of soil moisture
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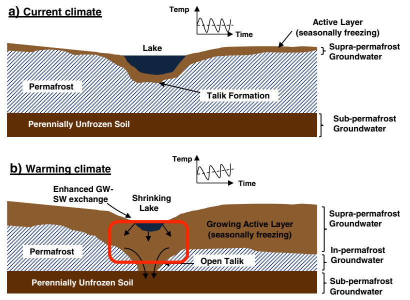
- Advective transport of energy
  - Will inclusion of advective energy transport significantly alter prediction of permafrost thaw?



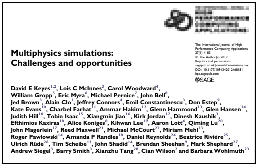
Kurylyk et al. (2014), Earth-Science Reviews

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



Multiphysics simulations: Challenges and opportunities

The International Journal of High Performance Computing Applications 27(1) 4–83
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DOI: 10.1177/1094342012468181
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David E Keyes[1,2], Lois C McInnes[3], Carol Woodward[4], William Gropp[5], Eric Myra[6], Michael Pernice[7], John Bell[8], Jed Brown[3], Alain Clo[1], Jeffrey Connors[4], Emil Constantinescu[3], Don Estep[9], Kate Evans[10], Charbel Farhat[11], Ammar Hakim[12], Glenn Hammond[13], Glen Hansen[14], Judith Hill[10], Tobin Isaac[15], Xiangmin Jiao[16], Kirk Jordan[17], Dinesh Kaushik[3], Efthimios Kaxiras[18], Alice Koniges[8], Kihwan Lee[19], Aaron Lott[4], Qiming Lu[20], John Magerlein[17], Reed Maxwell[21], Michael McCourt[22], Miriam Mehl[23], Roger Pawlowski[14], Amanda P Randles[18], Daniel Reynolds[24], Beatrice Rivière[25], Ulrich Rüde[26], Tim Scheibe[13], John Shadid[14], Brendan Sheehan[9], Mark Shephard[27], Andrew Siegel[3], Barry Smith[3], Xianzhu Tang[28], Cian Wilson[2] and Barbara Wohlmuth[23]

Keyes et al. (2011)

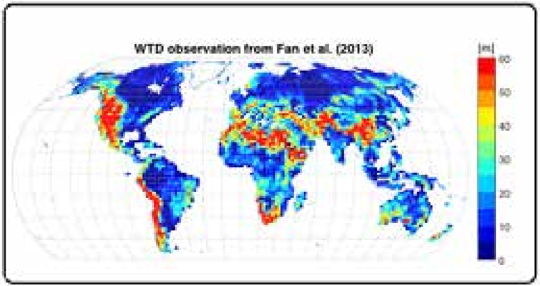
- Uses PETSc to provide numerical solution of discretized equations
- PETSc's `DMComposite` is used to solve tightly coupled multi-physics problems
- Open source available at `https://github.com/MPP-LSM/MPP`
- Follows an open development framework
- Using Travis-CI for testing on Linux and OS X
- Solution verification is being performed via method of manufactured solutions

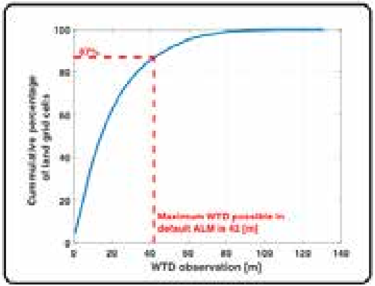
Outline

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_{drain}) had a dominant control on predicted water table depth (WTD)

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

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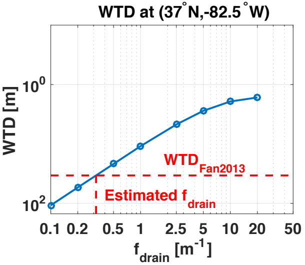
Simulation configuration:

- 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_{drain} values were performed for 200-years on $1.9^\circ \times 2.5^\circ$ grid to estimate an optimal f_{drain} for each grid cell
- A global simulation with optimal f_{drain} was performed for 200-years on $1.9^\circ \times 2.5^\circ$ grid

Estimation of f_{drain} parameter



Bisht et al. (2018) GMDD, in review

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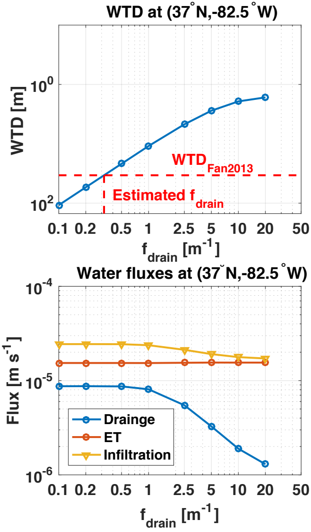

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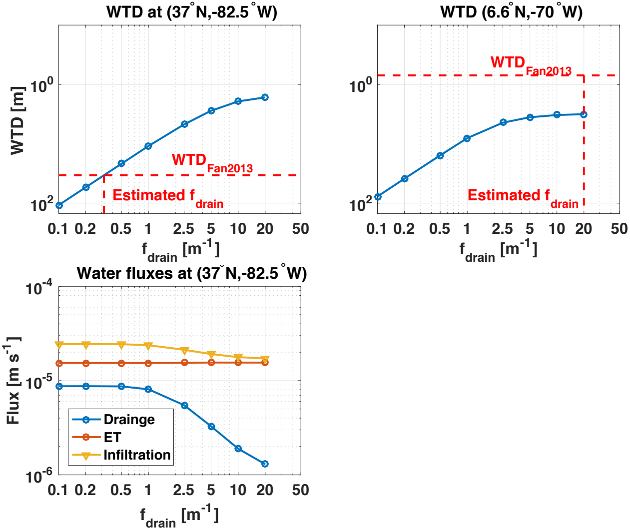

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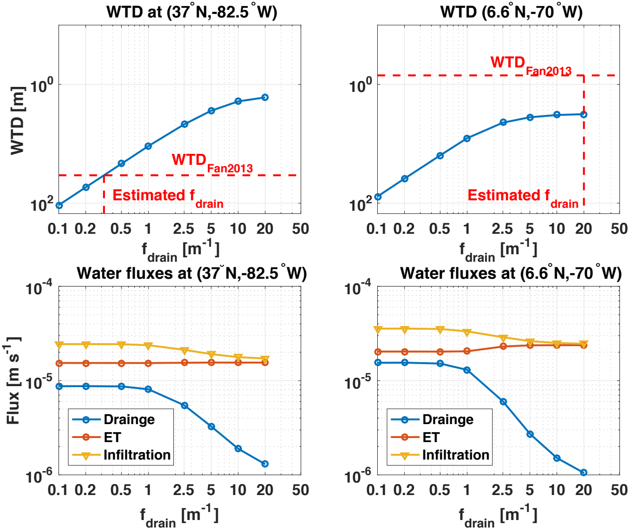
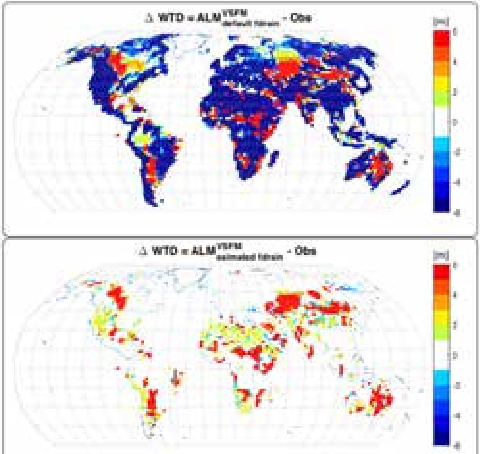


Bisht et al. (2018) GMDD, in review

Simulated water table depth anomalies



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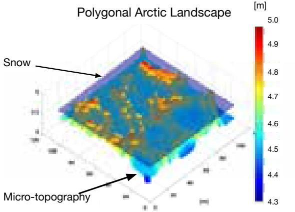
ELM with default f_{drain}			ELM with estimated f_{drain}		
Bias	RMSE	R^2	Bias	RMSE	R^2
-10.3	21.3	0.28	2.3	8.3	0.91

Lateral redistribution of heat in Arctic polygonal ecosystem

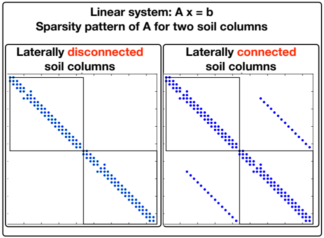
Objective:

- How spatial heterogeneity of soil temperature due to spatially variable snow depth is impacted by inclusion of lateral redistribution of heat?



Model:

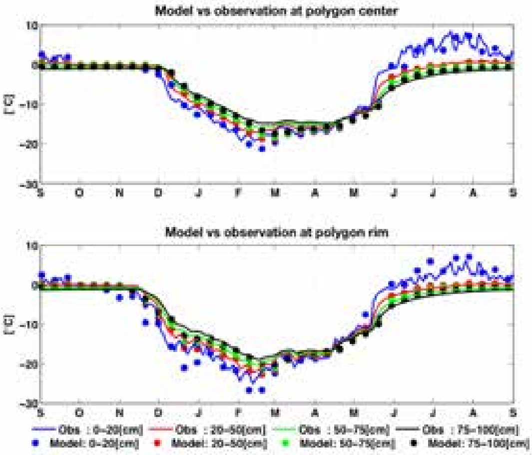
- Incorporated lateral energy transport in the subsurface within ELM.
- Spatial and temporal discretization leads to a set of linear equations that are solved via PETSc



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.

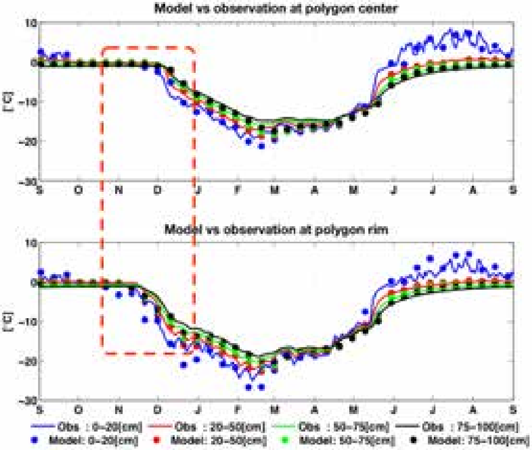
Simulated soil temperature profiles



Bisht et al. (2017), GMD

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

Simulated soil temperature profiles



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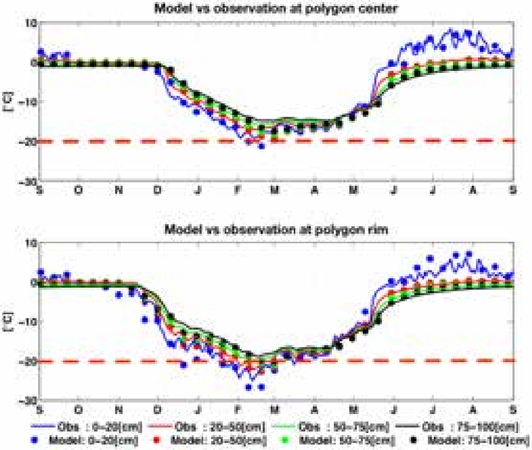

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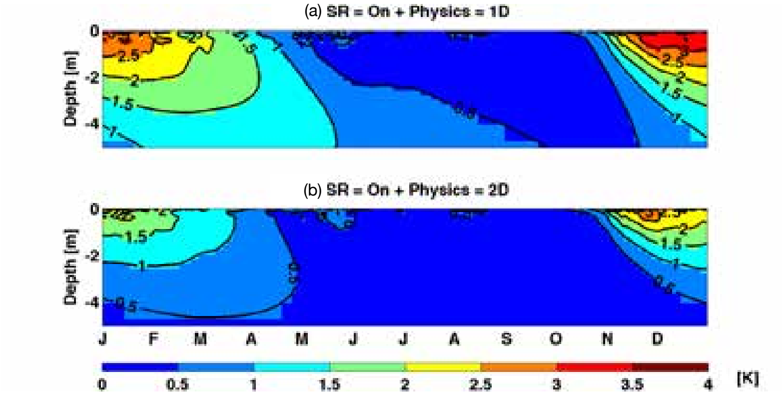
Simulated soil temperature spatial variability

Timeseries of spatial standard deviation for each soil layer averaged

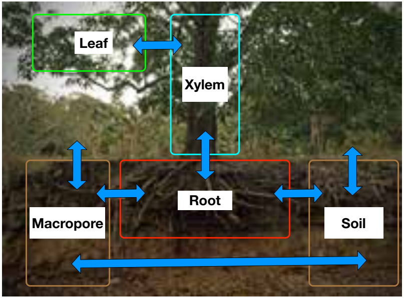


Bisht et al. (2017), GMD

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

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

$$\left(J_{s,s} \right) \left(\Delta X_s \right) = -\left(R_s \right)$$

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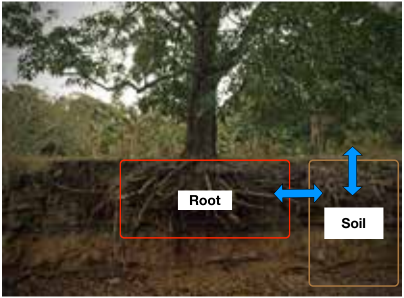

Solution of nonlinear equations for a soil-root system

$$\begin{pmatrix} J_{s,s} & J_{s,r} \\ J_{r,s} & J_{r,r} \end{pmatrix} \begin{pmatrix} \Delta X_s \\ \Delta X_r \end{pmatrix} = - \begin{pmatrix} R_s \\ R_r \end{pmatrix}$$

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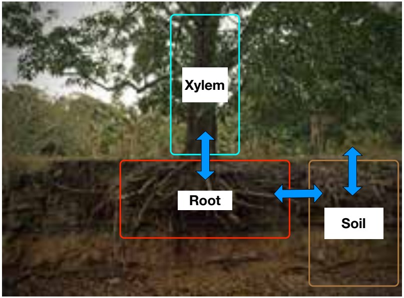
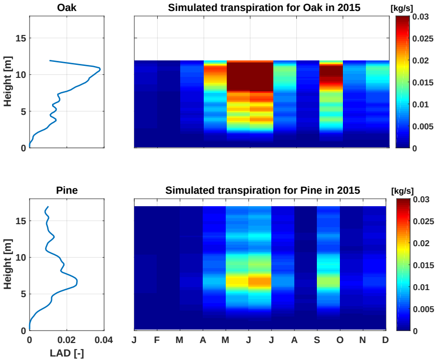


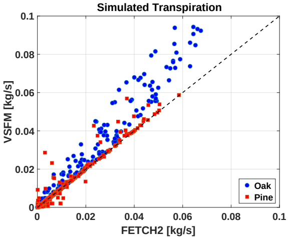
Solution of nonlinear equations for a soil-root-xylem system

$$\begin{pmatrix} J_{s,s} & J_{s,r} & 0 \\ J_{r,s} & J_{r,r} & J_{r,x} \\ 0 & J_{x,r} & J_{x,x} \end{pmatrix} \begin{pmatrix} \Delta X_s \\ \Delta X_r \\ \Delta X_x \end{pmatrix} = - \begin{pmatrix} R_s \\ R_r \\ R_x \end{pmatrix}$$

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?
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  Manufacture a solution:

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  $\lambda(x, y, z) = \exp(x + y + z - 1)$

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  Prescribe Q to each grid cell in the numerical model and solve for $T(x, y, z)$.

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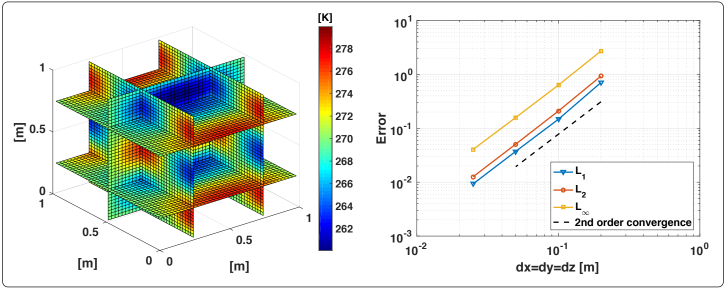

Thank you