Using Reactive Transport Codes to Provide Biogeochemistry Representations in Land Surface Models: Progress and Challenges with CLM-PFLOTRAN 1.0

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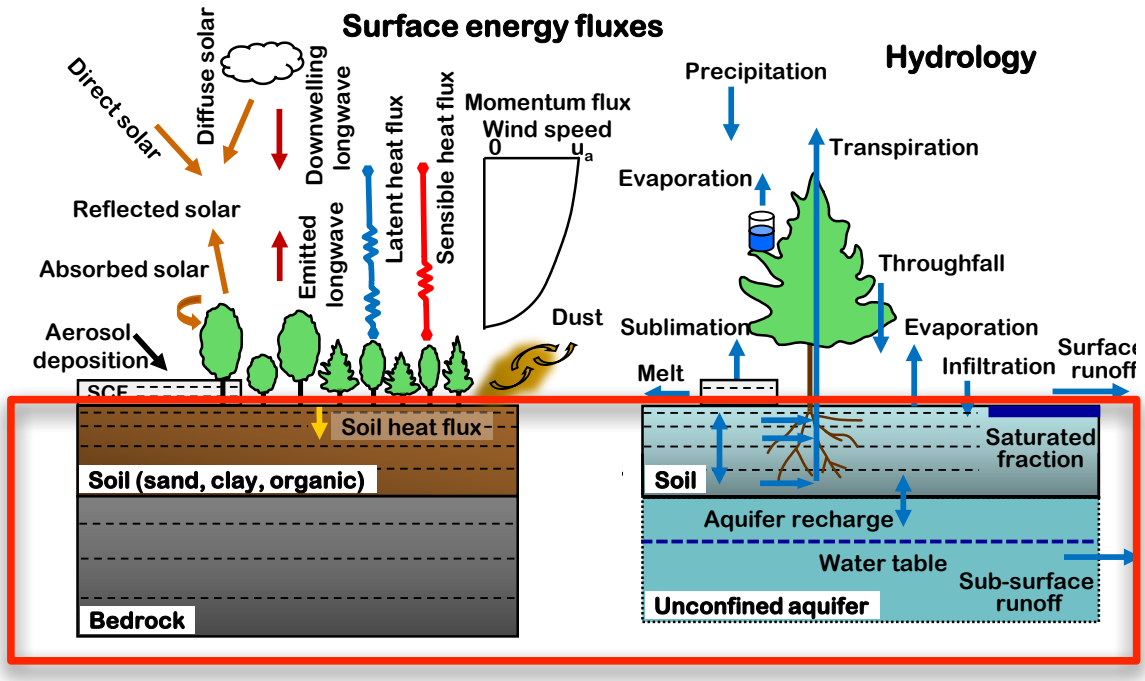
Credits and genesis of this work

- This work began as part of an 2012–2014 ORNL LDRD project for which I was PI. Goals were
  - Add surface-subsurface water interactions to PFLOTRAN.
  - Add freeze-thaw capability to PFLOTRAN (for permafrost thermal hydrology studies)
  - Couple CLM and PFLOTRAN, using PFLOTRAN for hydrology and below-ground biogeochemistry (processes in red box.)



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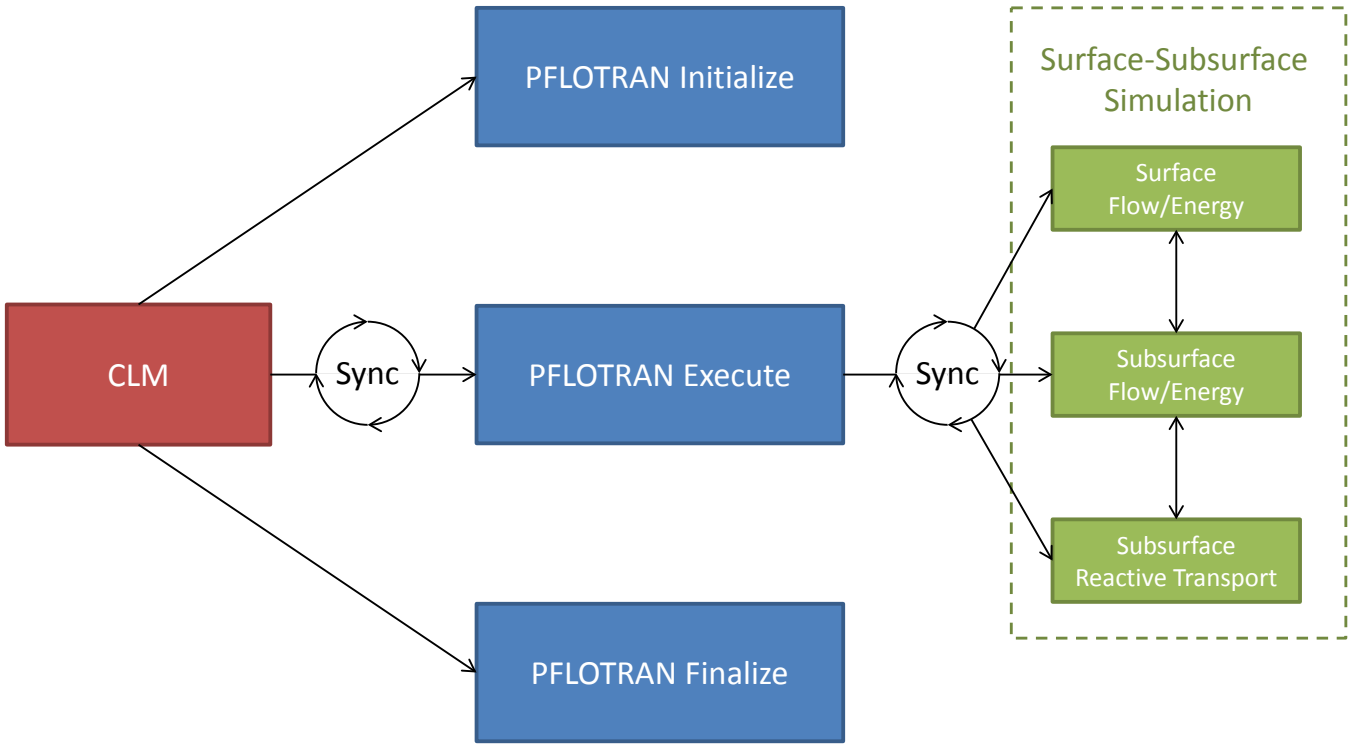
  - Couple CLM and PFLOTRAN, using PFLOTRAN for hydrology and below-ground biogeochemistry
- Gautam Bisht (now at LBNL) did heroic work on the project.
- Continued work by Guoping Tang and Fengming Yuan (among others at ORNL and elsewhere), with lots of PFLOTRAN help from Glenn Hammond (Sandia).
- See G. Tang et al., 2016, "Using reactive transport codes to provide biogeochemistry representations in land surface models: A proof of concept with CLM-PFLOTRAN 1.0", Geosci. Model Dev. Discuss., for details and full list of contributors. Also see Fengming Yuan's AGU 2015 poster abstract.

Reactive transport models in LSMs

- Land surface (terrestrial ecosystem) models (LSMs) generally hard-code soil biogeochemistry (BGC) reaction networks.
- To facilitate greater flexiblity and improve accuracy of solutions in BCG models, and to model fully 3D thermal hydrology and reactive transport, we have coupled CLM with the reactive transport code PFLOTRAN.
- In this talk, we will
  - Discuss some of the numerical challenges in making CLM and PFLOTRAN time stepping compatible.
  - Examine proof-of-concept tests with CLM-CN reaction network implemented in PFLOTRAN.
  - Show some results from using CLM-PFLOTRAN with 3D reactive transport to study soil N nutrient mobility effects on plant growth and SOM accumulation at the Barrow Environmental Observatory, Alaska.

CLM-PFLOTRAN coupling

- CLM "drives" and can instruct PFLOTRAN to solve PDEs for energy (including freeze-thaw), water flow, and reaction and transport in the surface and subsurface.



CLM-PFLOTRAN biogeochemistry coupling

- CLM "drives" and can instruct PFLOTRAN to solve PDEs for energy (including freeze-thaw), water flow, and reaction and transport in the surface and subsurface.
- Here, we implement the CLM-CN reaction network, initially focused on reaction (don't use PFLOTRAN transport until latter half of talk).
- At each CLM time step, CLM provides production rates for $\mathrm{Lit1C}$, $\mathrm{Lit1N}$, $\mathrm{Lit2C}$, $\mathrm{Lit2N}$, $\mathrm{Lit3C}$, $\mathrm{Lit3N}$ for litter fall; CWDC and CWDN for coarse woody debris production, N deposition and fixation, and plant N demand; and specifies liquid water content, matrix potential, and temperature for PFLOTRAN.
- PFLOTRAN solves ODEs for kinetic reactions and mass action equations for equilibrium reactions and passes final concentrations back to CLM.

PFLOTRAN reaction sandbox

- Reactions and rate laws are implemented using the "reaction sandbox" in PFLOTRAN.
- Isolates PFLOTRAN chemistry and provides simplified framework within which kinetic reactions can be rapidly implemented without having to completely learn the reaction process model.

```
subroutine SimpleReact(this,Residual,Jacobian,compute_derivative, &
                       rt_auxvar,global_auxvar,material_auxvar,reaction, &
                       option)
...
  ! multiplicative Monod w/biomass
  ! A + 2B -> C
  k = 1.d-7
  K_Aaq = 5.d-4
  K_Baq = 5.d-4
  stoichA = -1.d0
  stoichB = -2.d0
  stoichC = 1.d0
  Rate = k * Xim * Aaq / (K_Aaq + Aaq) * Baq / (K_Baq + Baq) * L_water
  RateA = stoichA * Rate
  RateB = stoichB * Rate
  RateC = stoichC * Rate
...
end subroutine
```


Mechanistic representation of rate-limiting processes

- CLM uses explicit time stepping with sequential coupling of processes; in PFLOTRAN we employ fully implicit time stepping for rigorous coupling of processes.
- Rate formulae designed for use in with explicit time stepping require modification to be made compatible with the fully implicit approach.
- E.g., CLM calculates plant and immobilization N demands independently of soil mineral N.
- Limitation of N availability on plant uptake and immobilization is simulated by demand-based competition (demands downregulated by soil N conc.)
- With implicit timestepping (full coupling), N limiting function must be added; we use a Monod substrate limitation function with half saturation k_m:

$$\frac{d[\mathrm{CN_u}]}{dt} = -k_{\mathrm{d}} f_{\mathrm{T}} f_{\mathrm{w}}([\mathrm{CN_u}] - [\mathrm{CN_u}]_{\mathrm{r}}) \frac{[\mathrm{N}] - [\mathrm{N}]_{\mathrm{r}}}{[\mathrm{N}] - [\mathrm{N}]_r + k_{\mathrm{m}}}, \qquad (1)$$

Avoiding negative concentrations

- Newton-Raphson iteration is the standard approach in PFLOTRAN to solve for an update vector $\delta \mathbf{c}^{k+1,p+1} = -\mathbf{J}^{-1}\mathbf{f}(\mathbf{c}^{k+1,p})$.
- Negative updates can lead to negative concentrations! Several approaches to deal with this:
  - Clipping: Limit the minimum concentration that can be modeled.
  - Scaling: Scale back updates with scaling factor λ: $\mathbf{c}^{k+1,p+1} = \mathbf{c}^{k+1,p} + \lambda\delta\mathbf{c}^{k+1,p+1} > 0$
  - Log transformation: Solve for update in log of concentration: $\delta \ln \mathbf{c}^{k+1,p+1} = -\mathbf{J}_{\ln}^{-1}\mathbf{f}(\mathbf{c}^{k+1,p})$
- First two options can introduce mass balance errors.
- Subtlety required in choosing appropriate approach. See GMDD paper for details.
- **Summary:** Log transformation is accurate and robust, but computational cost of clipping or scaling can be lower—though care must be taken in choosing tolerances.

CLM-PFLOTRAN: CLM-CN chemistry, Barrow, AK

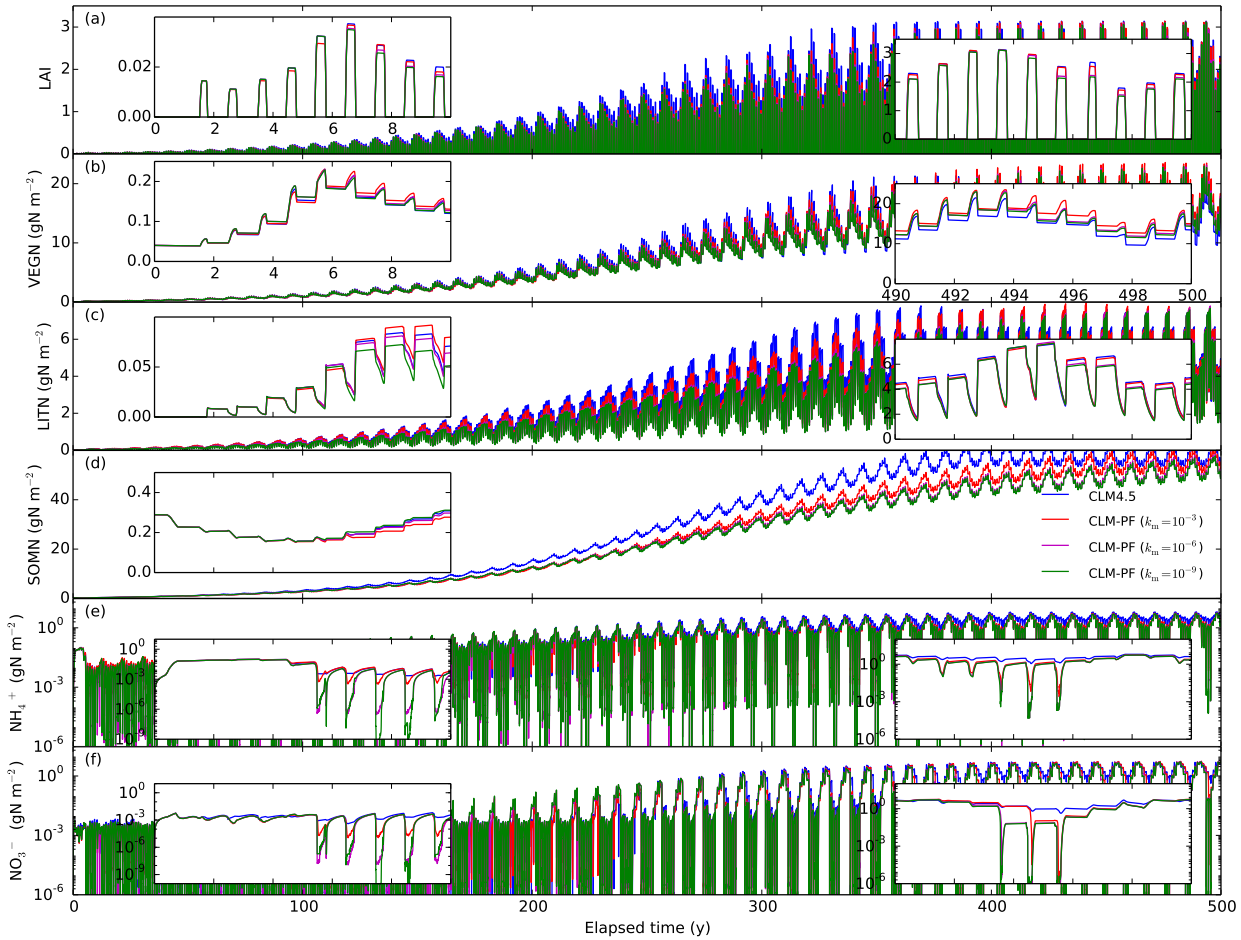
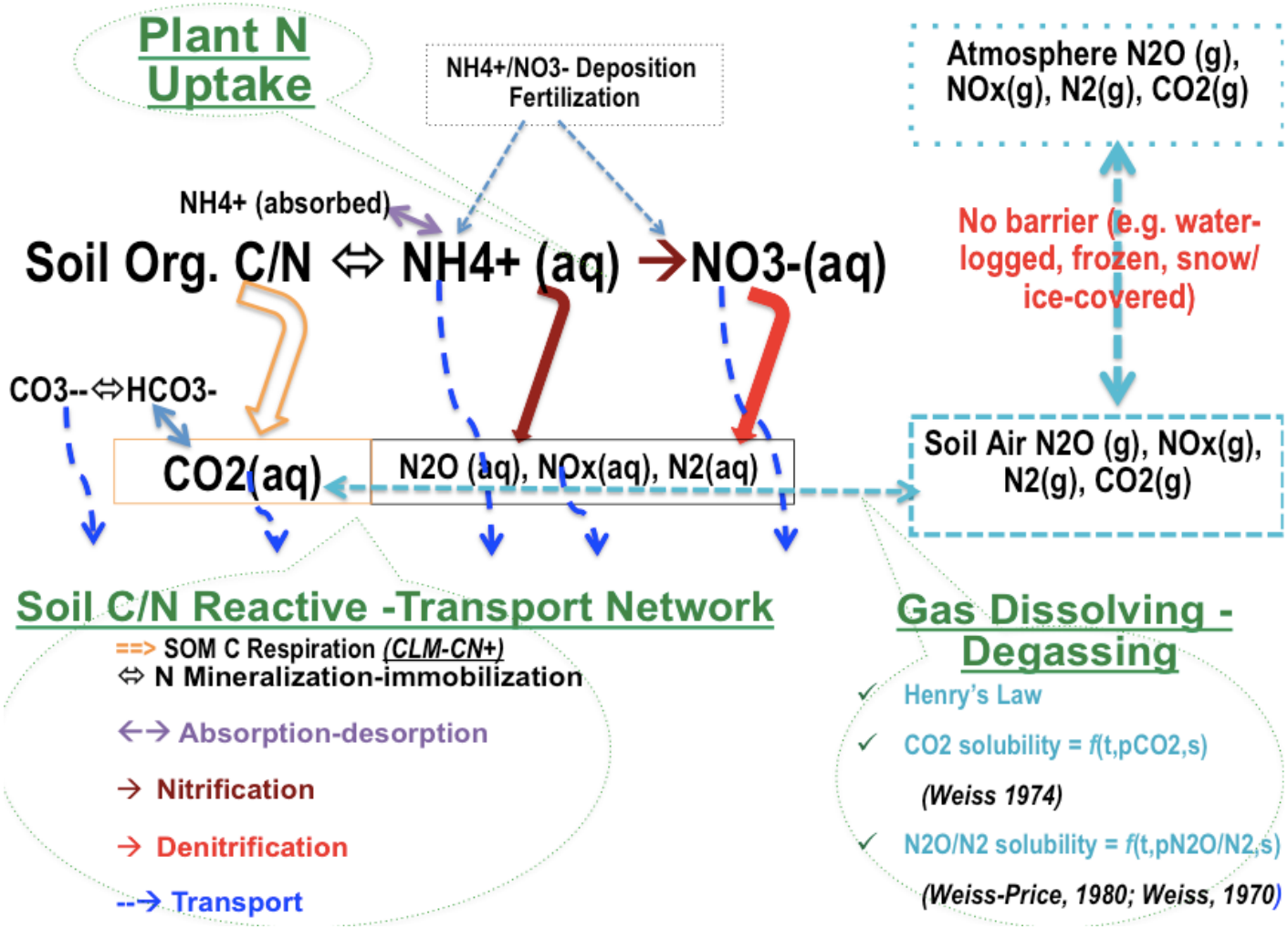


Figure: Calculated LAI and nitrogen distribution among vegetation, litter, SOM, NH_4^+, and NO_3^- pools in spin-up simulations for the Barrow, AK site. Small differences arise because 1) the N demand competition scheme implemented in CLM-PFLOTRAN is different from that in CLM4.5; 2) the former solves the reaction network simultaneously while the latter does so sequentially (resolves plant uptake and decomposition first, then nitrification, then denitrification); and 3) the C-N cycle is very sensitive to the N competition representation.

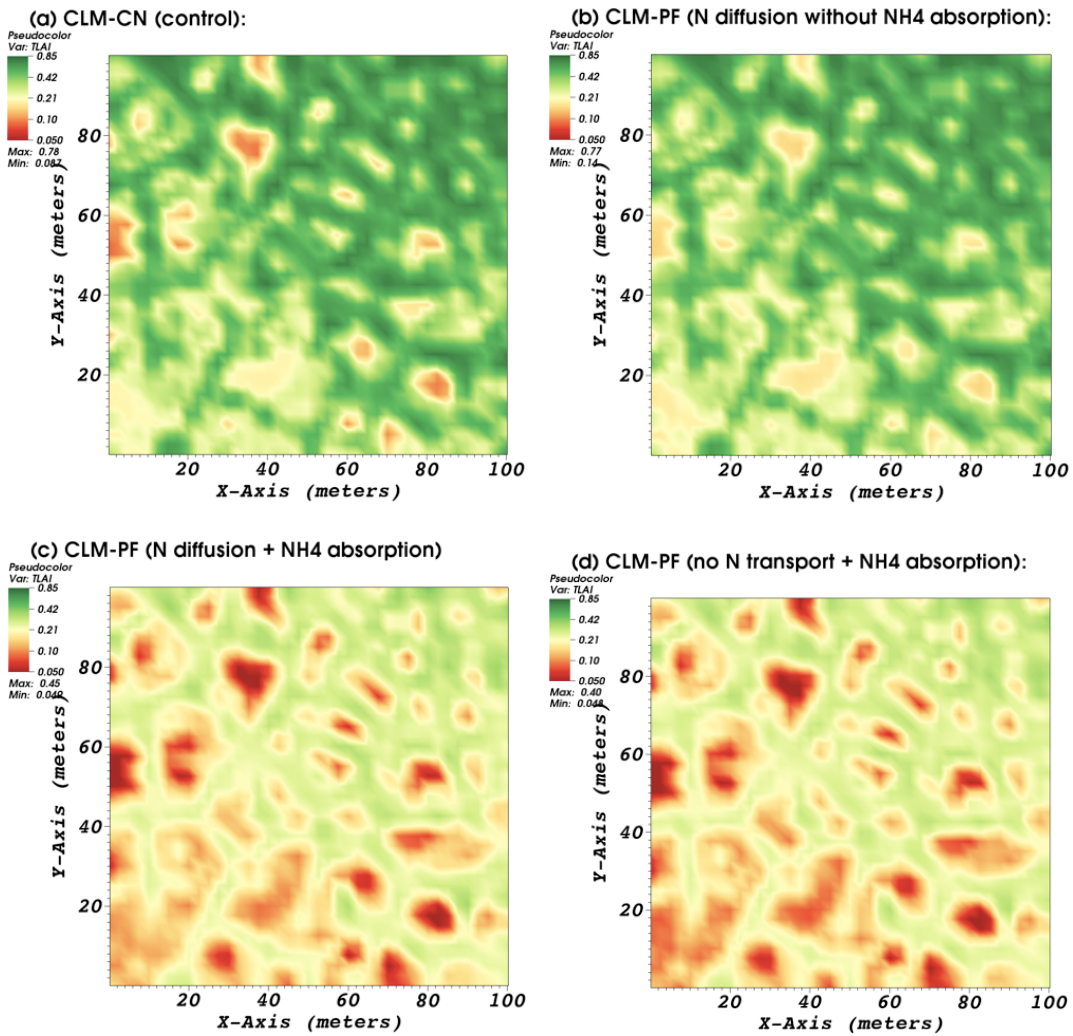
CLM-PFLOTRAN: C-N extended network



Extended C-N experiments, Barrow, AK

Simulations	NH4+ Absorption	Aq. NH4+/NO3- diffusion	Aq. NH4+/NO3- Advection
(a) CLM-CN (control)	NO	NO	With runoff & vertical drainage
(b) CLM-PFLOTRAN (test 1)	Turned OFF	Turned ON (3-D)	Turned OFF
(c) CLM-PFLOTRAN (test 2)	Turned ON	Turned ON (3-D or Vertical only)	Turned OFF
(d) CLM-PFLOTRAN (test 3)	Turned ON	Turned OFF	Turned OFF
(e) CLM-PFLOTRAN (test 4) (*in progress*)	Turned ON	Turned ON (3-D)	Turned ON *(with PFLOTRAN's Richards mode on)*

Extended C-N experiments: Effects on LAI



- (a) vs. (b): N diffusion (dispersion) in CLM-PFLOTRAN enables better plant growth in relatively low LAI areas in the CLM-CN model.
- (b) vs. (c): NH_4^+ absorption in CLM-PFLOTRAN constrains plant growth significantly. Without N transport as well (d), LAI is further decreased, but changes are small.

Figure: Comparison of total LAI ($\mathrm{m}^2\ \mathrm{m}^{-2}$) in August by (a) CLM-CN vs. (b)-(d) CLM-PFLOTRAN.

Extended C-N experiments: SOM C density

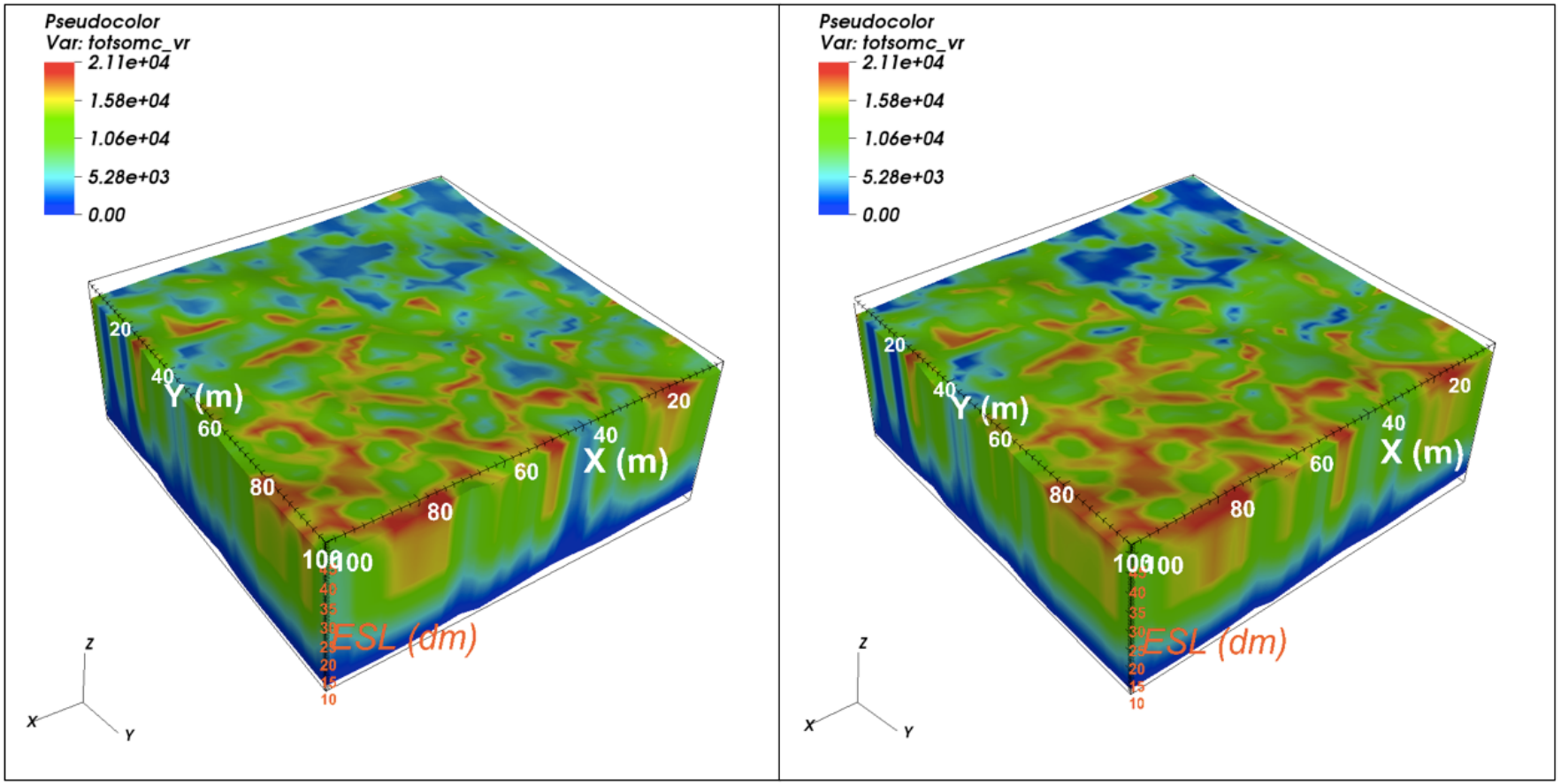


Figure: CLM-CN (left) and CLM-PFLOTRAN test 1 (right) simulated total SOM C density (100 g C m^{-3}) after accelerated spinup. Due to relatively better plant growth in regions such as polygon troughs in CLM-PFLOTRAN, CLM-PFLOTRAN simulates higher SOM C density in these regions.

Summary and Conclusions

- We have demonstrated the practicality of using a general-purpose reactive transport code inside CLM, closely reproducing the CLM-CN network as proof-of-concept.
- Implicit time stepping requires modifications to some reaction formulations and care to avoid some numerical issues, but allows tight coupling of processes, free from splitting errors and concerns about in what sequence to solve subproblems.
- It is relatively straightforward to implement new reaction networks using PFLOTRAN's reaction sandbox class.
- PFLOTRAN facilitates including 3D reactive transport, hydrologic, and thermal processes.
- CLM-PFLOTRAN simulation combining CLM-CN chemistry with soil NH_4^+ absorption processes and degassing-dissolving of C-N relevant greenhouse gas species suggest that soil N mobility significantly affects plant growth and thus long-term soil C stocks in permafrost-affected regions.

