Coupling a three-dimensional subsurface flow and transport model with a land surface model to simulate stream-aquifer-land interactions (CPv1.0) [MS No.: gmd-2017-35]

Responses to review comments

J. Kala (Editor) j.kala@murdoch.edu.au

This manuscript is well written. It describes the evaluation and coupling of CLM4.5, a widely used LSM, to PFLOTRAN, a subsurface model. The individual codes and model coupling are well described. The simulations are evaluated under real-life conditions. The paper fits the scope of GMD very well. The paper can be accepted following the following revisions:

The most major revision required to this paper is that results with CLM4.5 alone, without coupling to PFLOTRAN, are not presented. The reader hence does not get an idea of the added benefit of running the LSM coupled to a sophisticated subsurface model.

Response: We have added a CLM4.5 standalone simulation for comparison. Please see our response to the referee #1 for more details.

What are the differences in the surface heat fluxes by running CLM alone versus the coupled system? If sub-surface flows have an influence on the surface energy balance, then it needs to proved that it is actually worth the effort to run the coupled system?

Response: Please see the response to the question from Referee #1 above. The difference of subsurface flows on surface energy balance is significant between figure S4 (CLM4.5) and Figure 8(a) (i.e., CPv1) due to reasons stated in the response to Referee #1.

The abstract should mention the 3 different spatial resolutions used, especially as it is stated later that spatial resolution had a significant impact. In the abstract, it is also stated that including lateral subsurface flow impacted (I suggest using the word influenced rather than impacted) the surface energy budget and subsurface transport. How?

Response: Thanks for the constructive suggestions. We have added the spatial resolutions to the abstract, changed “impacted” to “influenced”, and added a phrase to discuss the reason why lateral subsurface flow could impact surface energy budget and subsurface transport. Please check the revised abstract for details.

At the end of the abstract, it is stated that this coupled system could be used to study land-atmosphere interactions. This is not really correct as this current modeling system does not *include a dynamic atmospheric component? You ran the model with prescribed meteorology. You cannot really make this conclusion.*

Response: Thanks. We have removed that sentence in the revised abstract.

Line 67 – The acronym ESM does not seem to be have previously defined? Is this acronym really necessary?

Response: Thanks. We have deleted the acronym ESM.

The introduction gives no indication why coupling CLM and PFLOTRAN is a good and worthwhile idea. Why these two models? If CLM has been coupled to other subsurface models such as PAWS, then what makes PFLOTRAN more advantageous than PAWS? While I have no doubt coupling CLM and PFLOTRAN is a great idea, you need to explain a bit more on why this is the case. Provide a bit more background, one paragraph should do.

Response: In response to this comment and that from the Referee #2, we have added literature reviews and discussions to elaborate the scientific motivation of this study (i.e., the potential of exploring the fully coupled aquifer-soil-vegetation-atmosphere continuum using an integrated model) in Section 1 of the revised manuscript. We also added discussions on how CP v1 differs from CLM-PAWS section 1 of the revised manuscript as follows:

"The developments of the integrated models have enabled scientific explorations of interactions and feedback mechanisms in the aquifer-soil-vegetation-atmosphere continuum using a holistic and physically based approach (Shrestha et al., 2014;Gilbert et al., 2017). Compared to simulations of regional climate models coupled to traditional LSMs, such a physically based approach shows less sensitivity to uncertainty in the subsurface hydraulic characteristics that could propagate from deep subsurface to free troposphere (Keune et al., 2016), while other physical representations (e.g., parameterizations in evaporation and transpiration, atmospheric boundary layer schemes) could have significant effects on the simulations as well (Sulis et al., 2017). Therefore, it is of great scientific interest to further develop the integrated models and benchmarks to achieve improved understanding of complex interactions in the fully coupled Earth system.

Motivated by the great potentials of using an integrated model to explore Earth system dynamics, the objective of this study is three-fold. First, we aim to document the development of a coupled land surface and subsurface model as a first step toward a new integrated model, featuring the two-way coupling between two highly-scalable and state-of-the-art open-source codes: CLM4.5 [*Oleson et al.*, 2013] and a reactive transport model PFLOTRAN [*Lichtner et al.*, 2015]. The coupled model mechanistically represents the two-way exchange of water and solute mass between aquifers and river, as well as land-atmosphere exchange of water and energy. The coupled model is therefore named as CP v1.0 hereafter. We note that in recent years, efforts have been made to implement carbon–nitrogen decomposition, nitrification, denitrification, and plant uptake from CLM4.5 in the form of a reaction network solved by PFLOTRAN to enable the coupling of biogeochemical processes between the two models [*Tang et al.*, 2016]. In addition, although PAWS is coupled to the same version of CLM (i.e., CLM4.5) (Ji et al., 2015;Pau et al., 2016), PFLOTRAN resolves the subsurface in a 3-D fashion, while PAWS approximates the 3D Richards equation by divide the subsurface into an unsaturated domain represented by the 1-D Richards Equation coupled with 3D saturated groundwater flow equation for subsurface flow, by assuming that there is no horizontal flow in unsaturated portion of soil, and that lateral flux in saturated portion is evenly distributed."

The paper tends to make use of many acronyms, and many of these do not seem necessary. Please only use acronyms where it is warranted. For example, the LEAF acronym is only used once, so there is no point in defining it if you don't use it again. Please carefully review all your acronyms.

Response: Thanks. We have deleted all unnecessary acronyms.

In Figure 1, some of the arrows do not seem to make sense to me. CLM links directly to PFLOTRAN Initialize, execute and finalize. Surely, CLM should only link to PLFOTRAN initialize, when then links to PFLOTRAN execute, then finalize. Also, according to your diagram, no information flows back from PFLOTRAN to CLM? Your diagram suggests that there is no two-way coupling? But the text state that soil moisture and hydraulic properties from PFLOTRAN and given back to CLM. Your flowchart does not really show this? Use m day-1 rather than m d-1.

Response: In response to all reviewers' comment regarding model coupling, we have significantly revised the technical details about model coupling in Section 2.3 (see below) and added a new schematic describing the model coupling (Figure 1). We have updated Figure 1 to better represent the two-way model coupling. We also have changed the unit "m d-1" to "m day-1".

"In this study, CLM4.5's one-dimensional models for flow in unsaturated (Zeng and Decker, 2009) and saturated (Niu et al., 2007) zones are replaced by PFLOTRAN's RICHRADS mode to simulate unsaturated-saturated flow within the three-dimensional subsurface domain. Although PFLOTRAN is also capable of simulating coupled flow and thermal processes in the subsurface including explicit representation of liquid-ice phase (Karra et al., 2014), as well as, soil nutrient cycles, (Hammond and Lichtner, 2010;Zachara et al., 2016;Tang et al., 2016), those processes are not coupled between the two models in this study. A schematic representation of the coupling between CLM4.5 and PFLOTRAN is shown in Figure 1. A model coupling interface based on PETSc data structures was developed to couple the two models and the interface includes some key design features of the CESM coupler [*Craig et al.*, 2012]. The model coupling interface allows each model grid to have a different spatial resolution and domain decomposition across multiple processors. While CLM4.5 uses a round-robin decomposition approach, PFLOTRAN employs domain decomposition via PETSc (Figure 1a). Interpolation of gridded data from one model onto the grids of the other is done through sparse matrix vector multiplication. As a preprocessing step, sparse weight matrices for interpolating data between the two models are saved as mapping files. Analogous to the CESM coupler, the mapping files are saved in a format similar to the mapping files produced by the ESMF_RegridWeightGen (https://www.earthsystemcog.org/projects/regridweightgen). ESMF regridding tools provide multiple interpolation methods (conservative, bilinear, and nearest neighbor) to generate the sparse weight matrix. In this work, we have used a conservative remapping method to interpolate data between CLM and PFLOTRAN. During model initialization, the model coupling interface first collectively reads all required sparse matrices. Next, the model coupling interface reassembles local sparse matrices after accounting for domain decomposition of each model (figures 1b and 1c). "

Figure 4 – Sorry I can hardly read any of the figure titles, please make these larger and more easily readable.

Response: Thanks for pointing this out. We have made the font of the figure titles bigger in the revised manuscript, including those in supplementary materials (figures S1 and S2).

Lines 359 – 361: You state that cold month were excluded from the analysis as you end up with division by zero issues when LH becomes close to zero. That's why most people use the evaporative fraction (EF), rather than the Bowen ratio. With EF, you take the ratio of latent to the sum of sensible and latent, hence, you will not have division by zero issues. You should use EF rather than Bowen ratio.

Response: Thanks for the great suggestion. We have redone the analysis using EF instead of Bowen ratio, and modified the figure and text in the revised manuscript correspondingly.

Section 4.1 – Please use model evaluation rather than model validation. Validation implies the model is already correct to start with and you are therefore validating it. This is of course never true of any model.

Response: Thanks for the great suggestion. We have changed the section title to be "Model evaluation".

Line 418: Looking at Figure 7(a) and 8, I find it hard to get an accurate idea of the differences, could you please plot the difference instead? Figure 10 – can you please remove the textbox at the bottom (CONTOUR FROM.......). Looks like an NCL plot to me
I'm sure you can remove this: ares@cnInfoLabelOn = False

Response: We have modified the figures as suggested. Please check the revised manuscript for details. We also modified the figures in the supplementary material accordingly to be consistent.

Line 447: Don't start a sentence with And. Your use of the 2 m simulation as a surrogate truth is fine, given a lack of observations of what is being simulated. However, you cannot really say simulation x outperformed simulation y (line 482), explain why one simulation appears more realistic, but I am not comfortable with the word "outperform". It would have been really interesting if you ran your model over a site for which observationally derived flux tower estimates of H and LE are available, such that you could then assess if this coupled system actually improves on CLM4.5 alone in simulating surface energy fluxes. I do understand that locations where Flux tower data are currently available (e.g., the FLUXNET network), may not necessarily be regions where the hydrology is interesting enough to warrant the use of such a model. You do however, need to acknowledge somewhere that the model needs to be evaluated against actual observations of surface fluxes.

Response: Thanks for the great suggestions. We have modified the sentences as suggested in the revised manuscript. In fact, two flux towers have been installed along the Hanford reach for this purpose but the analysis of the flux measurement is still preliminary. In addition, both towers are a little distant from the modeling domain to satisfy the requirements of eddy covariance measurements. Nevertheless, we also added discussions on the need of evaluating the model using eddy covariance measurements in section 5 of the revised manuscript.

Code availability: We had a recent discussion among GMD editors, and the point of the Code Availability section is to ensure the reproducibility. What we want is the exact code used for this paper. It is of course understandable that the code is still under development, however, we request you make the version of the code used for this paper available. If this is already on bitbucket or github, it is quite easy to make the revision/branch used for this study on ZENODO, which is the preferred repository for code as per GMD guidelines as it will generate an actual DOI for the code: http://www.geoscientific-model-development.net/about/code_and_data_policy.html
If you do a quick search on ZENODO, you will find several codes which point to github/bitbucket repositories, but a "frozen" version of the code used can be directly obtained from ZENODO, rather than a user having to work out which branch/revision of your code was used in the paper from the github/bitbucket repo

Response: Thanks for the instruction. The model and data have been made publicly available at

- https://bitbucket.org/clm_pflotran/clm-pflotran-trunk: CLM code
- https://bitbucket.org/clm_pflotran/pflotran-clm-trunk: PFLOTRAN code
- https://bitbucket.org/pnnl_sbr_sfa/notes-for-gmd-2017-35: Data

The README file in the notes-for-gmd-2017-35 repository provides detailed notes on how to create, compile, and run a simulation. Once the manuscript is accepted, we will start porting the frozen version of the code to ZENODO.

Reference:

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