Interactive comments on “Forward and inverse modeling of water flow in unsaturated soils with discontinuous hydraulic conductivities using physics-informed neural networks with domain decomposition” by Toshiyuki Bandai and Teamrat A. Ghezzehei

Reviewer comments are in black, while reply to comments in red.

The paper is very interesting and introduces a physics-informed neural networks (PINNs) method in a Richards’ equation context, aimed at approximating the solution to the RRE using neural networks while concurrently matching available soil moisture data. In particular, in this paper authors consider domain decomposition for handling infiltration into layered soils.

The topic is definitely up to date, the paper is well written, and provides all the details for implementing and understanding this approach. Nevertheless, I think authors should address some comments and issues before it can be accepted.

Response: We appreciate that the reviewer closely read our manuscript and gave the valuable comments. We would like to answer the questions below.

This PINN approach appears really fascinating because it allows to integrate physics-based models (such as RRE) with machine learning features. Authors ascribe the uncertainties in Richards’equation to the choice of boundary conditions, which is surely right. Nevertheless, I think they do not consider the (even more) cumbersome uncertainties arising from the choice of model parameters, which are the result of some non-linear fitting in laboratory experiments (I am referring to the parameters in the WRC and HCF). This point is a main concern for me: as a matter of facts, unsaturated flow dynamics strongly relies on functions parameters, rather than on ICs and BCs, which are generally easier to assess. On the other hand, I see authors already published a paper on this topic: I think it would be valuable to stress the differences between the two papers

Response: We appreciate your comments on the concern regarding the soil hydraulic parameters. We deeply acknowledge the effect of the uncertainty of the soil parameters on the soil moisture dynamics. From our previous study (Bandai and Ghezzehei, 2021), where we attempted to estimate the parameters from soil moisture measurements, we recognized the importance of understanding the basic characteristics of PINNs constrained by the RRE and its extension to layered soils for practical applications. In the revised manuscript, we will stress this point. In future studies, we will include the uncertainty of the parameters into this PINNs framework again.

Lines 197-198: few more words for sketching how the partial derivatives are computed would be valuable

Response: Thank you for pointing out that there needs more explanation on the automatic differentiation. In this method, all the computations necessary for PINNs are formulated as computational graphs by the software (TensorFlow in this study). Any derivatives related to the computations can be computed based on the reverse-mode automatic differentiation (basically, chain rule). The cost of computing the derivative is similar to or less than conducting the computation twice, regardless of the number of parameters. Therefore, this method is suitable for training neural networks with tens of thousands or millions of parameters. We will add an explanation of automatic differentiation in the revised manuscript.

Figure 1: I think there is a typo in the box “Physics and Data Constraints”, since the partial derivative at the left-hand side should be accomplished with respect to time.

Response: We regret to have left the typo in the figure. Thank you very much for noticing the mistake. We will fix this in the revised manuscript.

I understand that the residual is computed between the synthetic data and the computed (by the PINNs) ones; in this framework, what is the rationale of comparing the PINNs output with any Richards solver (as Hydrus)?

Response: The comparison with other RRE solvers (such as HYDRUS-1D) was conducted in the forward modeling, where we verified the ability of PINNs to approximate the solution to the RRE. It is important to make sure the performance of PINNs for the forward modeling because the performance of PINNs for the inverse modeling partially depends on the performance of the forward modeling.

As far as I understand, the power of this approach is to combine physics-based models with data driven ones; according to my knowledge, this is also the spirit of Data Assimilation (DA) methods, which incorporate measurements into a physics based model, albeit in a very different framework; these methods have also been treated in Richards' equation context (see for instance Berardi et al CPC https://doi.org/10.1016/j.cpc.2016.07.025, Medina et al HESS https://doi.org/10.5194/hess-18-2521-2014, Liu et al JoH https://doi.org/10.1016/j.jhydrol.2020.125210 ); what is authors' opinion about this? What would be the pros and cons of PINNs approach with respect to DA one? Also DA methods allow to assimilate boundary conditions, as in this case, and hydraulic parameters, as well as states. As a matter of fact, with respect to DA methods, this PINNs approach seems to me more on the theoretical side (which is definitely fine, of course) rather than application oriented.

Response: We appreciate that the reviewer pointed out the relation with data assimilation (DA). Our view is that both PINNs and DA are methods for inverse problems, where we aim to extract information from measurement data (Asch et al., 2016). We answer the questions by dividing DA methods into 3-D or 4-D variational methods (also called adjoint methods) and Kalman filter methods.

Adjoint methods are closely related to PINNs. In fact, we are currently working on the comparison between PINNs and adjoint methods. The difference comes from, for instance, the basis functions (linear functions for adjoint methods and neural networks for PINNs) and the method of minimizing the objective function. However, the methods might give very similar results based on our experiences. We would like to report this finding in future studies.

As the reviewer commented, the Kalman filter method might be more practical because it can also give an uncertainty of the results in addition to the point estimate. To the best of our knowledge, we are not aware of the comparison between the Kalman filter method and PINNs.

To conclude, our opinion is that all the methods mentioned here are within inverse modeling. The efficacy of each method would depend on the system of interest and the available data. As a research community, we need some benchmark problems to compare the methods.

Authors mention the possibility to drop loss terms for IC or BC at line 225. However, they have not presented any experiment for this scenario. Could you please comment on this ill-posed configuration? How would it perform with respect to classical solver?

Response: It might have been unclear in the current manuscript. The ill-posed setting was used for the inverse modeling, where no initial and boundary conditions were enforced, and only measurement data were used to train PINNs. In terms of classical solvers (finite difference or finite element), it is also possible to deal with such ill-posed settings by treating the missing information (e.g., initial condition) as inversion parameters and formulating the problem as inverse modeling. This type of inverse modeling is hard to implement in standard hydrology software (e.g., HYDRUS-1D) because the number of parameters can be very large. However, in geophysics or optimal control fields, it is common to deal with this inverse problem using adjoint methods (e.g., Petra and Stadler, 2011; we will add this literature to the revised manuscript).

Figure 11 and 3. Please replace "Fintie" with "Finite".

Response: Thank you very much for noticing the mistake. We will fix this in the revised manuscript.

Authors make use of synthetic data: I had hard times to find where the reference to used data is described. Of course the use of synthetic data is fine, but they should highlight it at the beginning of the paper. Moreover, could you please explain how your method of synthetic data generation could compare to real measurement data? In other words, how robust is your result with respect to outliers, sensor noise and other technical issues when it comes to real data?

Response: We appreciate that the reviewer pointed out that it was not clear if the data are synthetic in the current manuscript. We will emphasize that regard in the introduction of the revised manuscript. The robustness of the algorithm against the sensor noise was addressed by incorporating the Gaussian noise into the synthetic data used in the inverse modeling section (Line 559-560). The other technical difficulties (e.g., outliers and model errors) were not addressed in this manuscript. In the real setting, outliers should be removed and not be fed into the algorithm because the algorithm assumes soil moisture dynamics can be described by the Richardson-Richards equation. As for model errors, as long as they can be described by the Gaussian distribution, they can be interpreted as the Gaussian noise as in the current manuscript. For example, we did not consider the effect of hysteresis on soil moisture dynamics in this study. The model error due to hysteresis might be described by the Gaussian noise for wetting and drying situations. However, If there are biases that cannot be described by the Gaussian in the model error, we need to update the model by incorporating those processes as forms of mathematical equations.

References

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