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.

Comments on: Forward and inverse modelling of water flow in unsaturated soils with discontinuous hydraulic conductivities using physics-informed neural networks with domain decomposition.

Summary

This paper presents the results from a comprehensive study using PINNs as a forward and inverse numerical solution for the Richardson-Richards equation. They tested new approaches for applying the PINN method, including a layer-wise locally adaptative function intended to work with layered heterogeneous soil profiles. In addition, the authors compared their approach to well-known numerical solutions for the Richardson-Richards equation, namely Finite Difference and Finite Element Methods (FDM and FEM). The PINNs approach was also validated with soil moisture measurements performed in a soil column in controlled conditions.

The paper appears to be relatively novel, being the first application of PINNs to the Richardson-Richards equation (to my knowledge). The literature proposed and the figures presented are of high quality. I enjoyed reading the paper. The results are encouraging on the applications of PINNs to model hydrodynamics in porous media, even if it takes much more time when compared with the classical approaches. We don't need to impose well-known boundaries and initial conditions, which is attractive once they are difficult to obtain in field applications. The domain decomposition for the layered soils is also very promising. Even classical approaches such as FDM and FEM struggle with heterogeneous soil profiles. So, I think the PINNs with the domain decomposition did quite well in modelling the soil water dynamics in the soil column.

Response: We appreciate you spending time reading our preprint and giving us feedback. We would like to provide answers to your comments and questions.

Specific comments/questions (that should be addressed and commented before publication):

It would be interesting to test the inverse solution with soil matric potential measurements (data is available if needed).

Response: Thank you for pointing out the possibility of using water potential as data. It is not difficult to modify our codes to test the inverse solution with water potential measurements. In the study, we preferred volumetric water content over water potential because volumetric water content sensors are more reliable and cover a wider range of soil moisture conditions (as stated in lines 184-186). We conducted additional numerical experiments using water potential data from the same HYDRUS-1D simulation used in the inverse modeling in the main text, and the estimated surface water flux is comparable to the case using volumetric water content (see Figure 1 below). We will include this result

in the supplementary material in the next revision.



Figure 1. Inverse modeling to estimate surface flux from five water potential measurements in a layered soil ($z \in \{-1, -5, -9, -13, -17\}$ cm). The left figure shows the comparison between the true and PINNs' volumetric water content. The right figure shows the true and estimated surface water flux.

What is your opinion on going to 2 and 3D modelling? Could the domain decomposition proposed in the paper be applied to speed up 2 and 3D solutions? I think that would be the actual gain in this methodology. FEM applications for the fully 3D solution of Richardson-Richard's equation are still slow and have many complications with mesh, especially for large domains. This also applies to the boundary and initial conditions imposition.

Response: Thank you for your suggestions. Yes, the domain decomposition was indeed invented for speeding up PINNs for large-scale simulations by dividing spatial and temporal domains into smaller ones (Jaqtaq and Karniadakis, 2020). Although we presented results in only 1D to understand how PINNs behave, we are moving toward 2D and 3D simulations using PINNs.

What about non-Darcian conditions, macropore flow, very high clay content soils. Do you think the method could be applied?

Response: We appreciate your comments on those processes. A simple answer is "as long as we can describe those processes as mathematical equations, we should be able to simulate those processes using PINNs." Please think of PINNs as numerical solvers, such as finite difference and finite element methods.

The mathematical formulation of non-Darcy flow was proposed by Swartzendruber (1962), for instance, and this formulation can be implemented using PINNs. As for macropore flow, we believe we do not have a good mathematical model that can take into account the effects of macropore flow on the overall water flow (Nimmo, 2021). Thus, it is difficult to use PINNs for macropore simulation (same for traditional finite difference and finite element).

In terms of water flow in very high clay content soils (i.e., swelling soils), we believe we can simulate water flow in clay-rich soils that can shrink and swell. J. Philips and D. E. Smiles studied infiltration into swelling soils and provided the mathematical formulation of the processes (e.g., Smiles, 1974). Note that the water flow rate would be flow rate "relative to soil particles" in that case, and we need to take into account the change in porosity. Although these simulations are not common, such mathematical models exist, and thus we think we can apply PINNs to clay-rich soils.

What about root-water-uptake? How can this be included in your approach? There exist some analytical solutions for these problems (Yuan and Lu, 2005[1])

Response: I appreciate your comment and the literature you suggested. The answer to this question would be the same as the one before. As long as we have mathematical models for root-water-uptake, we can use PINNs to simulate as we do using finite difference and finite element methods. Since we have some root-water-uptake models (e.g., Feddes and Raats, 2004), we can include the plant-root water uptake as a sink term in the Richards equation and implement PINNs.

Do you think one day the PINNs could take over the classical approaches? What is limiting it?

Response: This is an important question. We do not see PINNs taking over the classical approaches in the future. We instead envision combining PINNs with classical approaches. For example, we can use a finite element solution for large-scale simulation with a coarse mesh size to train PINNs and later decrease "mesh size" (using more residual points) to get more refined solutions using PINNs, where the finite element method cannot be used due to a significant amount of degree of freedoms. The limitation of PINNs is the difficulty in training PINNs. However, we recently observed an exciting breakthrough in training PINNs, so we expect training PINNs to be more efficient and consistent in the future.

What about practical applications? Irrigation management or contaminant transport in the vadose zone.

Response: Thank you for commenting on practical applications. Current practical applications are to estimate rainfall estimations from soil moisture measurements (directly related to the inverse problem shown in the main text). As for irrigation management, we can formulate an inverse problem for irrigation management, where "desired soil moisture distribution" would be used to train PINNs to determine "required irrigation to achieve the desired soil moisture distribution." We might be able to use PINNs to locate the source of contaminant from measured contaminant data in the vadose zone by solving an inverse problem, where a sink term in a convective-dispersion equation is to be estimated. We would like to emphasize that those problems are all inverse problems, so PINNs and traditional approaches are both applicable.

Overall, the paper is well written. The sections are balanced, and the flow is good, making the paper enjoyable to read.

Response: We thank your constructive comments and feedback. We will include some of the answers here in the revised manuscript.

References

Feddes, R. A., & Raats, P. A. C. (2004). Parameterizing the soil - water - plant root system. In R. A. Feddes, G. H. de Rooji, & J. C. van Dam (Eds.), Unsaturated-zone modeling: Progress, challenges, and applications (pp. 95–141). Springer Netherlands.

Jagtap, A. D., & Karniadakis, G. E. (2020). Extended physics-informed neural networks (XPINNs): A generalized space-time domain decomposition based deep learning framework for nonlinear partial differential equations. Communications in Computational Physics, 28(5), 2002–2041. https://doi.org/10.4208/cicp.oa-2020-0164 Nimmo, J. R. (2021). The processes of preferential flow in the unsaturated zone. Soil Science Society of America Journal, 85(1), 1–27. <u>https://doi.org/10.1002/saj2.20143</u>

Smiles, D. E. (1974). Infiltration into a swelling material.pdf. Soil Science, 117(3), 140–147.

Swartzendruber, D. (1962). Modification of Darcy's law for the flow of water in soils. Soil Science, 93(1), 22–29.