A Framework for Data-driven multi-scale parameterizations in coupled porous media and free-flow systems

Edward Coltman¹, Martin Schneider¹, Rainer Helmig¹

¹) Institute for Modeling Hydraulic and Environmental Systems, University of Stuttgart Edward.Coltman@iws.uni-stuttgart.de

Presented is a framework for the data-driven determination of multi-scale parametrizations for coupled porous media and free-flow systems.

Simulations of coupled flow and transport can become very complex when realistic applications are considered [1, 2]. Evaluations of these systems at the REV scale, although efficient when using model discretization methods [5], require well defined parameters that represent pore-scale phenomena to maintain their accuracy. Determining the optimal parameters for this often require expensive pore-scale calculations [6]. This work outlines a series of four steps where these parameters can be calculated, as outlined in Figure 1, and further explained in [3].

First, evaluations of a system are evaluated at the pore scale. Next, these solutions are averaged and evaluated in comparison to REV scale models with closure or dispersion terms. The calculation of optimal parameters minimizing the difference between these scales can then be generalized using a specialized convolutional neural network. Finally, the results and physical meaning of these parameterizations can be further investigated using a correlation analysis to descriptive pore metrics. All simulations are performed using the numerics simulator $DuMu^{x}$ [4].

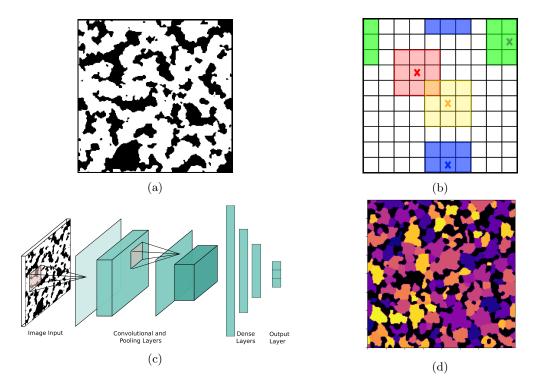


Figure 1: Framework outline: (1a) Pore-scale simulations, (1b) Averaging and closure term evaluation, (1c) generalizations via a CNN, (1d) evaluation of descriptive metrics.

References

- L. M. Bahlmann, K. M. Smits, K. Heck, E. Coltman, R. Helmig, and I. Neuweiler. Gas component transport across the soil-atmosphere interface for gases of different density: Experiments and modeling. *Water Resources Research*, 56(9):e2020WR027600, 2020.
- [2] E. Coltman, M. Lipp, A. Vescovini, and R. Helmig. Obstacles, interfacial forms, and turbulence: A numerical analysis of soil-water evaporation across different interfaces. *Transport in Porous Media*, 134:275–301, 2020.
- [3] Edward Coltman, Martin Schneider, and Rainer Helmig. A dumux framework for data-driven multi-scale parametrizations. arXiv, 2023.
- [4] T. Koch, D. Gläser, K. Weishaupt, S. Ackermann, M. Beck, B. Becker, S. Burbulla, H. Class, E. Coltman, S. Emmert, T. Fetzer, C. Grüninger, K. Heck, J. Hommel, T. Kurz, M. Lipp, F. Mohammadi, S. Scherrer, M. Schneider, G. Seitz, L. Stadler, M. Utz, F. Weinhardt, and B. Flemisch. DuMux 3 – an open-source simulator for solving flow and transport problems in porous media with a focus on model coupling. *Computers* & Mathematics with Applications, 2021.
- [5] M. Schneider, D. Gläser, K. Weishaupt, E. Coltman, B. Flemisch, and R. Helmig. Coupling staggered-grid and vertex-centered finite-volume methods for coupled porous-medium free-flow problems. *Journal of Computational Physics, Accepted, in Production*, 2023.
- [6] B. D. Wood, F. Cherblanc, M. Quintard, and S. Whitaker. Volume averaging for determining the effective dispersion tensor: Closure using periodic unit cells and comparison with ensemble averaging. *Water Resources Research*, 39(8), 2003.