Using a pore-network model to couple mass, momentum and energy at the interface between free flow and porous media flow

Kilian Weishaupt^{1*} and Rainer Helmig¹

Micro Abstract

Coupled systems of a porous medium with an adjacent free flow appear in a wide range of industrial and environmental processes. We propose an efficient coupled model comprising three domains: a bulk porous medium (Darcy's or Forchheimer's law) at the bottom, the free flow domain (Navier-Stokes) on the top and the interface region (dynamic pore-network model) in between. This model can help to provide effective upscaled parameters required for other mechanical modeling approaches.

¹Department of Hydromechanics and Modelling of Hydrosystems, University of Stuttgart, Stuttgart, Germany ***Corresponding author**: kilian.weishaupt@iws.uni-stuttgart.de

Introduction

Systems of coupled free flow and porous-medium flow appear ubiquitously in nature and in technical applications. Common examples for interface-driven transport and exchange processes include soil evaporation [9], fuel cell water management [3] or food drying [10].

Modeling these kinds of coupled systems on the pore scale (e.g. by means of DNS) is very often unfeasible due to the highly complex geometry of the porous material.

In contrast to that, REV-scale approaches describe the porous medium, including the region close to the interface to the free flow, only in an averaged sense. While providing the possibility to model larger domains, pore-scale effects like local saturation distribution patterns can often not be captured in sufficient detail. Theses effects, however, strongly affect the global behavior of the coupled system (see e.g [9]).

1 A concurrent hybrid multi-scale model

1.1 Concept

Here, we propose a novel method to tackle the issue of resolving the interface region between free flow and porous medium in ample detail, thereby accounting for pore-scale effects relevant for the overall system behavior, while maintaining a comparatively low computational effort which allows the simulation of rather realistic scenarios [8]. The key feature of this approach is a pore-network model [6] which represents the transition region between the porous matrix and the free flow. The final model will consist of three computational domains (see Fig. 1): the free-flow region where the (Navier-) Stokes equations are solved, the aforementioned transition zone described by the pore-network model and a bulk porous domain accounted for by Darcy's or Forchheimer's law. Appropriate coupling conditions ensure the continuity of mass, momentum and energy fluxes as well as thermodynamic consistency between the respective subdomains.



Figure 1. Conceptual scheme of the novel coupled model consisting of a free-flow region (Stokes), an interface region (pore-network model) and the bulk porous medium (Darcy).

1.2 Discretization and implementation

The (Navier-) Stokes equations applied for the free-flow domain are discretized in space using a staggered grid approach [4] where scalar quantities like pressure and density are located on the cell centers while the velocities are stored on the cell faces.

For the pore-network model used for the interface region, all balance equations are formulated per pore-body, while the fluxes occur within the one-dimensional pore throats.

The box method [5] is used to spatially discretize the balance equations of the REV-scale bulk domain. This approach combines the local mass-conservation properties of a finite-volume scheme with ansatz-functions known from finite-element methods, thereby enabling flexible and convenient spatial interpolation of discrete values which is important for the coupling.

A fully-implicit backward Euler scheme is used for the temporal discretization of all equations. All models are implemented in DuMu^x [2], an open-source simulation toolbox for porous media which is built upon DUNE [1], an open-source numerical framework for scientific applications. Apart from the DUNE core modules, dune-foamgrid [7] is required to provide an one-dimensional grid implementation for the pore-network model.

The three sub-models will be coupled in a monolithic approach, which means that all balance equations are assembled into one (potentially nonlinear) system of equations and solved simultaneously. This work is currently in progress, therefore only the coupling of two models (free flow to pore-network model or REV-scale to pore-network model) has been realized yet. Furthermore, for the time being, only isothermal single-phase flow is considered. This will be extended in future work.

2 First Results

2.0.1 PNM-Darcy coupling

Fig. 2 shows an exemplary setup for the coupling of the interface region (pore-network model, top of left figure) and the REV-scale bulk porous medium (bottom). Fixed pressures of $p_{top} = 0.99 \times 10^5$ Pa and $p_{bottom} = 1 \times 10^5$ Pa are set as Dirichlet boundary conditions at the top and bottom of the respective sub-domains, leading to a flux in upward direction. All other external boundaries are closed (Neumann no-flow). The permeability **K** of the bulk porous medium has been determined by numerical upscaling of the pore-network properties.

The evolution of pressure in vertical direction through both domains is depicted on the right hand side of Fig. 2. As imposed by the coupling conditions, a continuity of pressure at the interface between the two domains can be observed. Furthermore, the pressure gradient within both domains is identical as a result of the upscaled value of \mathbf{K} .



Figure 2. Exemplary coupling of a pore-network model (interface region, top) and a REV-scale model (bulk domain, bottom). The plot on the right indicates the continuity of the pressure itself and its identical gradient within the two domains.

2.0.2 PNM-Stokes coupling

The following example demonstrates the coupling of the interface region to the free flow. Water passes through a free-flow channel with an adjacent porous structure at low flow velocities (Re < 1). The free-flow channel has a length of approximately 50 mm and height of 2 mm. The porous structure has a total size of $10 \text{ mm} \times 10 \text{ mm}$, with square-cut pillars $(0.25 \text{ mm} \times 0.25 \text{ mm})$ arranged to a regular grid where the spacings between the pillars are also 0.25 mm.



Figure 3. Velocity fields of the reference solution (left) and the coupled model (right).

Fig. 3 shows that the solution of the coupled model fits very well with the one obtained by discretizing the complete domain in high detail.

Conclusions

This work provides the basis for the development of a hybrid-scale model capable of effectively describing coupled processes of free-flow and flow through a porous medium. Especially within the context of multi-phase flow, the pore-network model can help to capture local pore-scale effects otherwise inaccessible to classical REV-scale models. The concept may furthermore help to understand and quantify relevant interface-related phenomena which can then be transferred to other models e.g. by means of upscaling.

Acknowledgements

The authors would like to thank Alexandros Terzis, Guang Yang, Bernhard Weigand and Majid Hassanizadeh for their substantial support and fruitful discussions.

References

- P. Bastian, M. Blatt, A. Dedner, C. Engwer, R. Klöfkorn, M. Ohlberger, and O. Sander. A generic grid interface for parallel and adaptive scientific computing. Part I: Abstract framework. *Computing*, 82(2):103–119, 2008.
- [2] B. Flemisch, M. Darcis, K. Erbertseder, B. Faigle, A. Lauser, K. Mosthaf, S. Müthing, P. Nuske, A. Tatomir, M. Wolff, et al. DuMux: DUNE for multi-{phase, component, scale, physics,...} flow and transport in porous media. *Advances in Water Resources*, 34(9):1102–1112, 2011.
- [3] V. Gurau and J. A. Mann. A critical overview of computational fluid dynamics multiphase models for proton exchange membrane fuel cells. SIAM Journal on Applied Mathematics, 70(2):410–454, 2009.
- [4] F. H. Harlow and J. E. Welch. Numerical calculation of time-dependent viscous incompressible flow of fluid with free surface. *The Physics of Fluids*, 8(12):2182–2189, 1965.
- [5] R. Huber and R. Helmig. Node-centered finite volume discretizations for the numerical simulation of multiphase flow in heterogeneous porous media. *Computational Geosciences*, 4(2):141–164, 2000.
- [6] Y. Mehmani and M. T. Balhoff. Bridging from pore to continuum: A hybrid mortar domain decomposition framework for subsurface flow and transport. *Multiscale Modeling & Simulation*, 12(2):667–693, 2014.
- [7] O. Sander, T. Koch, N. Schröder, and B. Flemisch. The dune foamgrid implementation for surface and network grids. arXiv preprint arXiv:1511.03415, 2015.
- [8] T. D. Scheibe, E. M. Murphy, X. Chen, A. K. Rice, K. C. Carroll, B. J. Palmer, A. M. Tartakovsky, I. Battiato, and B. D. Wood. An analysis platform for multiscale hydrogeologic modeling with emphasis on hybrid multiscale methods. *Groundwater*, 53(1):38–56, 2015.
- [9] E. Shahraeeni, P. Lehmann, and D. Or. Coupling of evaporative fluxes from drying porous surfaces with air boundary layer: Characteristics of evaporation from discrete pores. *Water Resour. Res*, 48(9), 2012.
- [10] P. Verboven, D. Flick, B. Nicolaï, and G. Alvarez. Modelling transport phenomena in refrigerated food bulks, packages and stacks: basics and advances. *International Journal of Refrigeration*, 29(6):985–997, 2006.