

Hybrid multi-scale modeling of reactive transport in fractures— An adaptive embedded-boundary approach

Sergi Molins, Lawrence Berkeley National Laboratory,
David Trebotich, Lawrence Berkeley National Laboratory,
Bhavna Arora, Lawrence Berkeley National Laboratory,
Hang Deng, Lawrence Berkeley National Laboratory,
Carl Steefel, Lawrence Berkeley National Laboratory

Key words: Multiscale, Reactive transport, Fractures, Modeling, Embedded boundary, Adaptive mesh refinement, Chombo-Crunch, CrunchFlow

Understanding fracture evolution is essential in many subsurface applications, including subsurface storage, shale gas production, fracking, CO₂ sequestration, and geothermal energy extraction. Geochemical processes play a significant role in the evolution of fractures through dissolution-driven widening, fines migration, and/or fracture sealing due to precipitation. Conceptually, fractured systems have been represented as being composed of fast flow paths -the fractures- and slow flow paths - the rock matrix.

Darcy-scale continuum models have treated fractures as preferential flow paths with their permeability evolving as a function (often, a cubic law) of the fracture aperture. This approach has the limitation that it may oversimplify flow within the fracture and the geochemical reaction parameters as well-mixed conditions need be assumed in each grid cell of the model. In contrast, pore scale models make it possible to resolve the fracture surface geometry explicitly in three dimensions and solve for flow and reactive transport within the pore space of the fracture. The model can capture the channelization of the flow path due to dissolution in transport limited conditions. However, even with high performance computing, the pore scale model is still limited in their ability to treat finer-scale heterogeneity that falls below the resolution of the discretization.

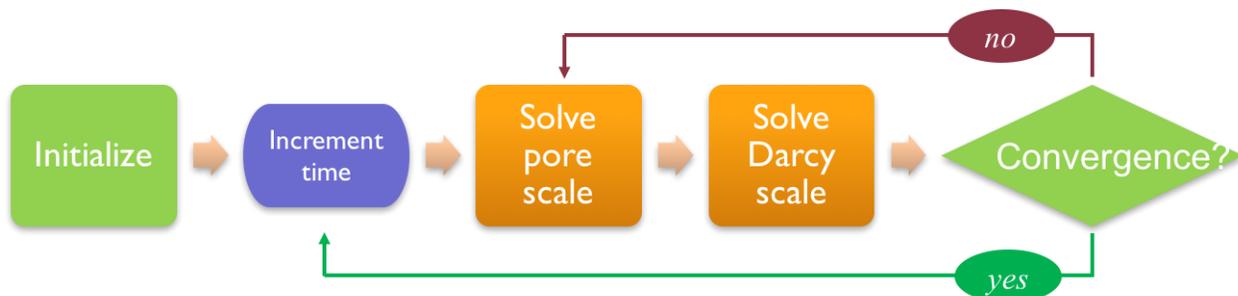


Figure 1: Multiscale coupling approach

In this contribution, we extend the previously developed pore scale model Chombo-Crunch [1-4] to include a porous continuum that captures fine scale processes within the rock matrix while keeping a pore scale representation of the fracture itself. The resulting multi-scale model is capable to simulate flow and reactive transport within a tortuous fracture geometry using a pore-scale approach and a porous matrix using a Darcy-scale approach. Computationally, both domains are connected via explicit flux matching (*Figure 1*) across an interface represented by an embedded boundary in a structured mesh framework. The embedded boundary method also makes it possible to capture the complex pore space geometries in natural subsurface materials.

Further, we utilize the adaptive mesh refinement (AMR) capabilities available in the software framework Chombo [5]. AMR is a numerical technique for locally adjusting the resolution of computational grids that makes it possible to superimpose levels of finer grids on the global computational grid in an adaptive manner allowing for more accurate

calculations locally [6]. Here, we use AMR to accurately capture concentration gradients that develop in localized areas of the simulation domain, while using a coarser grid elsewhere.

We use recent observations from a fractured core experiment [7] to demonstrate the features of the model. In particular, we accurately evaluate the relative importance of transport limitations to reactive surfaces due to (1) the development of diffusive boundary layers at the pore scale and (2) the tortuosity of the porous medium at the Darcy scale.

References

- [1] Molins, S., Trebotich, D., Steefel, C. I., & Shen, C. (2012). An investigation of the effect of pore scale flow on average geochemical reaction rates using direct numerical simulation. *Water Resources Research*, 48(3), doi.org/10.1029/2011WR011404
- [2] Molins, S., Trebotich, D., Yang, L., Ajo-Franklin, J. B., Ligoeki, T. J., Shen, C., & Steefel, C. I. (2014). Pore-Scale Controls on Calcite Dissolution Rates from Flow-through Laboratory and Numerical Experiments. *Environmental Science & Technology*, 48(13), 7453–7460. doi.org/10.1021/es5013438
- [3] Molins, S., Trebotich, D., Miller, G. H., & Steefel, C. I. (2017). Mineralogical and transport controls on the evolution of porous media texture using direct numerical simulation. *Water Resources Research*. <https://doi.org/10.1002/2016WR020323>
- [4] Trebotich, D., Adams, M. F., Molins, S., Steefel, C. I., & Shen, C. (2014). High-Resolution Simulation of Pore-Scale Reactive Transport Processes Associated with Carbon Sequestration. *Computing in Science & Engineering*, 16(6), 22–31. <https://doi.org/http://dx.doi.org/10.1109/MCSE.2014.77>
- [5] M. Adams, P. Colella, D. T. Graves, J.N. Johnson, N.D. Keen, T. J. Ligoeki, D. F. Martin, P.W. McCorquodale, D. Modiano, P.O. Schwartz, T.D. Sternberg and B. Van Straalen, *Chombo Software Package for AMR Applications - Design Document*, Lawrence Berkeley National Laboratory Technical Report LBNL-6616E.
- [6] Dubey, A., Almgren, A., Bell, J., Berzins, M., Brandt, S., Bryan, G., ... Weide, K. (2014). A survey of high level frameworks in block-structured adaptive mesh refinement packages. *Journal of Parallel and Distributed Computing*, 74(12), 3217–3227. doi.org/10.1016/j.jpdc.2014.07.001
- [7] Deng, H., Molins, S., Steefel, C., DePaolo, D., Voltolini, M., Yang, L., & Ajo-Franklin, J. (2016). A 2.5D Reactive Transport Model for Fracture Alteration Simulation. *Environmental Science & Technology*. <https://doi.org/10.1021/acs.est.6b02184>