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# Sub-grid Modeling in a Particle-based Approach: Regularization of Non-linear Hyperbolic Conservation Law

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Conventional numerical modeling techniques, with finitely resolved length and time scales, need specific treatments to include the effects of unresolved physics and solution discontinuities. In this regard, their applications to multi-scale problems involving transport in fractured media are no different. Lagrangian particle-tracking methods provide a compelling alternative to the Eulerian methods as they provide a natural connection across a multitude of scales. Further, in the context of purely advective transport, the absence of numerical diffusion makes them better placed to capture solution discontinuities, if any.

In this work, we present a stochastic particle-based framework which models reactive multiphase transport in porous media characterized by highly conductive fractures and a permeable matrix. Thereby, we use an Embedded Discrete Fracture Model (EDFM) where large fractures are resolved with lower dimensional representations [Deb and Jenny, (2017)] Macroscopic transported quantities, e.g., phase-saturation, are modeled in the essence of particle ensemble statistics.

We present a flux-conservative stochastic particle-tracking scheme tailored to EDFMs, and we illustrated its applicability for advective solute transport. Therein, we devised the probability of inter-continuum particle transfer which is particle trajectory-specific. Further, we extended this scheme to model saturation evolution in two-phase flows. Solutions of the opted non-linear hyperbolic transport problems involve discontinuities. Hence, we added minimal diffusion to the system, and to this end, an adaptive diffusion coefficient is proposed. It is inspired by the Smagorinsky-model [Smagorinsky (1963); Lilly (1966)] developed in the context of Large Eddy Simulations of turbulent flows, and it is active only in the vicinity of a saturation fronts, and thus is not overly diffusive.

The new particle-tracking scheme correctly captures the sharp saturation profiles of 1-D Buckley-Leverett problems. It is shown how the adaptive diffusion coefficient can be generalized for a wide range of flow scenarios including those with buoyancy. As a part of this exercise, comparisons of 2-D particle-based solutions are compared with those from a suitable Eulerian approach. Eventually, the capability of the overall framework for a large-scale fracture model is assessed. Subsequent research includes modeling of sub-grid processes, e.g., dissolution of one phase into the other [Tyagi (2011)] and liquid phase-solid matrix interactions. This warrants, once again, a probabilistic approach to model the transitions of particles in the state space.

## Participation

In-Person

## References

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