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Modeling interfaces explicitly with an embedded-boundary finite-volume method across applications

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Porous media are characterized by their physical and chemical heterogeneity at a range of length scales. As a result, the interfaces between the different phases or materials present in the media are complex. Processes near or at these interfaces often exert a controlling effect on the outcome of applications in which these porous media are used. Process-based modeling is a powerful tool to understand how the different processes interact to produce the observed behavior. However, representation of these interfaces in models in order to capture the relevant processes explicitly remains a challenge.

In this presentation, we describe an embedded-boundary method that enables us to incorporate interfaces explicitly in a block-structured finite-volume model. In this approach, the irregular domain created by complex interfaces is discretized as a collection of control volumes formed by the intersection of the problem domain with the cubic Cartesian grid cells, as in a "cut cell"approach. The various operators are approximated by applying the divergence theorem on the irregular control volumes, with the fluxes computed by using primary discretized dependent variables that approximate the solution evaluated at the centers of the original Cartesian cells. Away from the boundary, the finite-volume method reduces to a standard finite-difference approximation.

We demonstrate the approach in three applications to reactive transport in porous media. In all cases, we consider fluid flow, solute transport, aqueous complexation and mineral dissolution-precipitation reactions. The applications cover a range of conceptual models. We start with an application where the interfaces separate fluid and solid phases and reaction rates are limited by solute transport to the interfaces. We follow with fractured media, where interfaces separate the fracture opening from the surrounding matrix. In this case, transport limitations exist both in the fracture as well as in the matrix. We end with an application to reverse osmosis where the interface acts as a permeable boundary to water but not to ions in solution.

Participation

In-Person

References

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