Algorithmic solution of a two-scale hybrid discrete-continuum model for transport, biofilm development and solid restructuring

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Processes related to the formation, stability, and turnover of soil microaggregates act on various spatial scales. While the reactive transport of species in a porous medium is efficiently described at the continuum (meso)scale, the restructuring of aggregates in the μm range requires a discrete model on the pore scale (microscale), see [1].

The appropriate description of these processes and the combination of the scales leads to algorithmic and numerical challenges. We present a numerical approach for the treatment of such a coupled mechanistic two-scale model to account for the interplay of geochemistry and microbiology, and the link to soil functions as the porosity, e.g.

At the pore scale reactive transport within different phases including diffusion, advection, drift (emerging from electric forces), and growth and decay of biofilms are formulated in terms of a continuous PDE-ODE-AE framework. The solution strategy is fully implicit using the local Discontinuous Galerkin method. The above effects interfere with the evolution of the porous structure (the aggregates) in space and time that is realized in the discrete setting of a cellular automaton. The resulting model is upscaled with techniques of mathematical homogenization to gain effective parameters for flow and transport on the mesoscale. The microscale and upscaling problems rely on versatile combinations of cellular automata and discontiuous Galerkin methods while on the mesoscale mixed finite elements are used.

[1] Ray, Rupp, Prechtel (2017) *Goldschmidt Abstracts.*