Hybrid discrete-continuum modeling for reactive transport, biofilm development and solid restructuring

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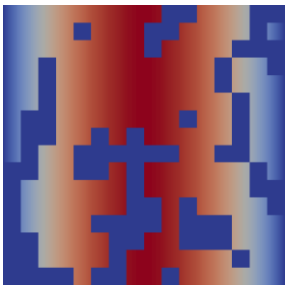
We present the mathematical, mechanistic modeling of processes leading to the formation, stability, and turnover of soil microaggregates. This aims at deterministic aggregation models including detailed mechanistic pore scale descriptions to account for the interplay of geochemistry and microbiology, and the link to soil functions.

We consider both processes at the pore scale and at the scale of the soil microaggregate (mesoscale). At the pore scale transport by diffusion, advection, and drift emerging from electric forces can be taken into account, in addition to homogeneous and heterogeneous reactions of species in a continuous PDE setting. Additionally, in the context of soil micro-aggregates, the growth of biofilms and glueing substances such as EPS (extracellular polymeric substances) plays an important role since they affect the structure of the pore space in space and time (see Fig. 1). These aspects are implemented within a discrete cellular automaton approach. The resulting model is upscaled to transfer it to the mesoscale. The upscaled model describing the effective transport and fluid flow contains effective time- and space-dependent coefficient functions. These functions may be explicitly computed by means of auxiliary cell problems that are defined in time- and space-dependent representative pore scale geometries. The numerical simulations allow studying



the interplay between the considered processes and their link to soil functions.

Figure 1: Artifical example for combination of (continuous) evolution of reactive species and coupled (discrete) evolving particles (from [1]).

[1] Ray, Rupp, Prechtel (2016) *Preprint Series Angewandte Mathematik* Nr. 393, University of Erlangen, 48p.