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Discrete-continuum multiscale model for evolving microaggregates in porous media

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Microaggregates are the fundamental building blocks of soils and thus important for its structure, properties and functions. Although there has been much research on the links, dynamics, stability, and structure of soil microaggregates, there is still a substantial lack of quantifying the relationships between the key factors of their dynamics. Those key factors are soil fauna, microorganisms, roots, inorganics, and physical processes [Totsche et al. 2017]. We assess the complex coupling of biological, chemical and physical processes at different scales with the help of a mechanistic modeling approach in order to gain a model-based mechanistic understanding of the formation, build-up, composition, properties and stability of microaggregates.

Our dynamic framework combines biomass development and structural changes in the solid originating from stabilizing sticky agents or electric effects in a comprehensive micro-macro model [Ray et al. 2017]. It uses a versatile discrete cellular automaton method (CAM) on the microscale with a continuous PDE formulation on the micro and the macroscale. This means that the underlying time-dependent computational domain for the pore scale, i.e. the distribution of a solid, biomass, a wetting, and a non-wetting fluid is determined discretely by means of a CAM. The diffusion of mobile bacteria, possibly transforming into immobile biomass, nutrients, and ions are prescribed by means of PDEs, likewise, the surface concentration of a sticky agent tightening together solid or bio cells (in the cellular automaton context) is considered. The idea of using a CAM setting with biofilm growth at the pore scale goes back to work in [Tang / Valocchi, Tang et al].

To omit the explicit tracking of interfaces as it is necessary in level-set approaches we use this combined discrete-continuum approach. As the soil is evolving in this setting we have to use a discretization for the PDE systems in the fluid that is robust and handles discrete discontinuities. The local discontinuous Galerkin (LDG) method is suitable for this task.

One main objective of this research is to examine the strong interplay between functional properties and geometric structure. To that end standard homogenization results are used to compute the soil's characteristic properties such as porosity or effective diffusion tensors for the resulting complex and time-dependent geometries.

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