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Linking processes to structure and structure to function: Hybrid discrete-continuum modeling for microaggregate formation

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We present the development and application of a mathematical, mechanistic model to describe and analyse processes related to the formation of soil micro-aggregates. It combines formulations at two scales: the pore scale and the macroscale.
Firstly, a discrete cellular automaton model on the pore scale takes into account building units of different sizes, shapes, charges, and glueing properties. They can recombine and move in a fluid including reactive solutes and biomass. The reactive transport of the solutes is realized in a partial differential equation setting. We study the interplay between processes as electrostatic attraction, or types of building units, on the resulting structures in a systematic way by analysing, e.g. different ranges of attraction. The structure is analysed with the help of geometric measures such as compactness or connectivity.
Secondly, the link of the evolving microstructure to resulting functions of the soil is provided by upscaling the equations on the microscale to the macroscale with the help of (periodic) homogenization techniques resulting in effective, time and space depending coefficients/parameters for the resulting complex and time-dependent geometries, e.g. effective diffusion tensors.
Simulations also complement aggregation experiments for goethite, illite and quartz and address questions of homoaggregation, and heteroaggregation of different particles.