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Simulating Structure Formation in Soils across Scales using Discontinuous Galerkin Methods

Simulation von Strukturbildung im Boden auf unterschiedlichen Skalen mithilfe unstetiger Galerkin–Verfahren

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This thesis deals with mathematical modeling, analysis, and numerical realization of microaggregates in soils. These microaggregates have the size of a few hundred micrometers and can be understood as the fundamental building units of soil. Thus, understanding their dynamically evolving, three-dimensional structure is crucial for modeling and interpreting many soil parameters such as diffusivities and flow paths that come into play in CO2-sequestration or oil recovery scenarios.

Among others, the following aspects of the formation of microaggregates should be incorporated into a mathematical model and investigated in more detail: the spatial heterogeneity of the temporally evolving structure of microaggregates and the different processes that take place on different scales—temporal and spatial—within the so-called micro-scale itself. This work aims at formulating a process-based pore-scale model, where all chemical species are measured in concentrations. That is, we have a continuous model for reactive transport mainly in terms of partial differential equations (PDEs) with algebraic constraints. This continuous model is defined on a discrete and discretely moving domain whose geometry changes according to the rules of a cellular automaton method (CAM). These rules describe the restructuring of the porous matrix, growth and decay of biomass, and the resulting topological changes of a wetting fluid and a gas phase. The cellular automaton rules additionally imply stochastic aspects that are important on the pore-scale.

Moreover, effects and knowledge deduced from the model are transfered to scales which are more relevant for applications. The quality of these averaged models is of general interest, since simulations for the field-scale that resolve the pore-scale are not applicable for economical reasons. Thus, this book compares parameterizations of diffusivities with mathematically rigorous results and gives suggestions to improve the formulas that can be found in the literature.

The discrete movement of the microaggregates' geometry at the micro-scale poses mathematical problems. The following question arises: Can the averaged quantities deduced from the pore-scale really be used for models on other scales or are the impacts of the artificial temporal jumps too detrimental for the solutions on other scales to be accurate? In the following, this problem is also dealt with, and the reliability of the obtained parameters is underlined.

Last but not least, it is imperative to apply a proper numerical method to implement the model in silico. The local discontinuous Galerkin (LDG) method seems to be suitable for this task, since it is locally mass-conservative and is stable for discontinuous data—that might, for example, originate from the discrete movement of the geometry or from the sharp boundaries between the different phases. Additionally, this method has no problems with complicated transfer conditions. These aspects are demonstrated in a mathematically rigorous way, and the method is improved upon by reducing the linear system of equations resulting from the discretization. This is a real enhancement, since it does not diminish the order of convergence but decreases the computational costs.