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Upscaling flow and transport properties in synthetic porous media

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Flow and transport through the porous media has instances in nature and industry: contaminant migration in geological formations, gas/oil extraction from proppant filled hydraulic fractures and surrounding porous matrix, underground carbon dioxide sequestration and many others. We would like to understand the behavior of propagating solute front in such medium, mainly flow preferential pathways and the solute dispersion due to the porous medium geometry. The motivation of our investigation is to find connection between the effective flow and transport properties and porous media geometry in 2D and 3D for large system sizes. The challenge is to discover a good way of upscaling flow and transport processes to obtain results comparable to these calculated on pore-scale in much faster way.

We study synthetic porous media made of densely packed poly-disperse disk-or spherical-shaped grains in 2D and 3D, respectively. We use various protocols such as the random sequential addition (RSA) algorithm to generate densely packed grains. Imposed macroscopic pressure gradient invokes fluid flow through the pore space of generated porous medium samples. As the flow is considered in the low Reynolds number regime, a stationary velocity field is obtained by solving the Stokes equations by means of finite element method. Void space between the grains is accurately discretized by using body-fitting triangular or tetrahedral mesh. Finally, pure advection of a front carried by the velocity field is studied. Periodicity in all directions is applied to microstructure, flow and transport processes.

Effective permeability of the media can be calculated by integrating the velocity field on cross sections, whereas effective dispersion coefficient is deduced by application of centered moment methods on the concentration field of transported solute in time. The effective parameters are investigated as a function of geometrical parameters of the media, such as porosity, specific surface area and fractal dimension of the pore space geometry. Discretization effects are taken into account.

Furthermore, as we aim to simulate transport processes in complex and large systems in 3D, following upscaling technique is checked against the original calculations. The pore space of the media is approximated in the form of a capillary network by converting the pore space throats between the grains into lines in 2D and polygons in 3D. Effective flow and transport properties are calculated on such network models and compared with the results obtained for original geometry.