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Let's move to spheres! Why a spherical coordinate system is rewarding when analyzing particle increment statistics

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For understanding non-Fickian transport in porous media, thorough understanding of pore-scale processes is required. When using particle methods as research instruments, we need a detailed understanding of the dependence and memory between subsequent increments in particle motion. We are especially interested in the dependence and memory of the spatial increments (size and direction) at consecutive time steps. Understanding the increment statistics is crucial for the upscaling that always becomes essential for transport simulations at larger scales. Upscaling means averaging over a (representative elementary) volume to save limited computational resources. However, this averaging means a loss of detail and therefore dispersion models should compensate for this loss. Formulating an appropriate dispersion model requires a detailed understanding of the dependencies and memory effects in the transport process. Particle-based simulations for transport in porous media are usually conducted and analyzed in a Cartesian coordinate system. We will show that, for understanding the process physically and representing the process statistically, it is more appropriate to switch to a spherical coordinate system that moves with each particle.

Increment statistics in a Cartesian coordinate system usually reveal that a large displacement in longitudinal direction triggers a large displacement in transverse direction as fast flow channels are not perfectly aligned with the Cartesian axis along the main flow direction. We can overcome this inherent link, typical for the Cartesian description by using the absolute displacements together with the direction of the particle movement, where the direction is determined by the angles azimuth and elevation. This can be understood as a Lagrangian spherical process description.

The root of the dependence of the transport process is in the complex pore geometry. For some time past, high-resolution micro-CT scans of pore space geometry became the basis for extremely realistic transport simulations at the pore-scale. Based on such a highly resolved simulation, we derive the highly-nonlinear dependence structure over a range of scales. Further, we analyze the dependence structure of the transport processes under varying influence of diffusion. The increment statistics of a special coordinate system combined with a copula-based analysis gives a comprehensive picture of the transport processes for different Peclet numbers, and over different scales.