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A cross-platform, high-performance SPH toolkit for image-based flow simulations on the pore scale of porous media

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Efficient numerical simulations of fluid flow on the pore scale allow for the numerical estimation of effective material properties of porous media like effective permeability or tortuosity, among others. In contrast to time-consuming and often expensive laboratory tests, pore scale-resolved numerical simulations further enable the computational quantification of anisotropy of inherent material properties and the estimation of representative sample domains. Numerically calculated quantities are valuable in several fields, such as carbon dioxide sequestration, geothermal energy production and groundwater contamination remediation. Our specific pore scale-resolved simulation method directly based on images obtained from Micro X-Ray Computed Tomography (μXRCT) is based on the weakly compressible Smoothed Particle Hydrodynamics (SPH) approach. SPH is a meshless Lagrangian method, highly suitable for modeling complex geometries and flow at moderate Reynolds numbers. Low Reynolds number flow, also denoted as creeping flow, is a typical scenario present in the above mentioned applications. However, SPH is computationally demanding, especially in simulations of large domains. To overcome these difficulties, we have designed a specific SPH module for the highly optimized HOOMD-blue Molecular Dynamics software. Our implementation supports single-phase flow, and targets both CPU and GPU clusters. Due to the high computational demands, scalability is essential to make the software practically usable, and our tests indicate that our implementation can scale almost ideally. We study a wide variety of test cases, which are not only representative for XRCT-based geometries, but for pore scale-resolved flow simulations in general. Additionally, we present a large-scale simulation investigating an unconventional high porous volcanic rock sample (Reticulite).

REFERENCES

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