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Exploring with simulations the transport properties of multi-scale porous materials

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The internal structure of many natural porous materials such as soils and carbonate rocks involves multiple length scales. This severely hinders the research relating structure and transport properties: typically laboratory experiments cannot distinguish contributions from individual scales while computer simulations cannot capture multiple scales due to limited computational resources. 3D imaging and image-based fluid flow simulations are increasingly used for studying the pore-scale transport processes. Combining imaging with pore-scale flow simulation techniques, e.g. the lattice Boltzmann method, provides direct means to quantify pore-scale transport processes. However, pore-scale computer simulations have not really been able to capture multiple scales due to the limited size of the simulation system.

We show here that the current computational resources and software techniques already allow transport simulations in domains beyond the realms of current imaging techniques, and, more importantly, enable numerical experiments in multi-scale porous materials. We were able to simulate single-phase fluid flow with the lattice Boltzmann method in a synthetic x-ray-tomography image taken from the set of world's largest 3D images of a porous material [1]. The used image has 16384^3 image voxels and porosity of 0.134 (i.e., $5.9 \cdot 10^{11}$ pore voxels) and it represents the microstructure of Fontainebleau sandstone. While the modelled sandstone image is rather homogeneous and therefore does not really represent a multiscale porous material, from a computational point of view it serves the purpose of demonstrating the power of contemporary software and hardware techniques. The simulation was executed at the Edinburgh Parallel Computing Centre on the ARCHER supercomputer ranked number 25 among all supercomputers. ARCHER has 3008 computing nodes each of which has two 12-core Ivy Bridge 2.7 GHz CPUs and 64 GB of memory providing 1.67 Petaflops of theoretical peak performance. The simulation was executed using 2880 nodes (96% of the total node count) and the steady-state was reached after 20000 discrete time steps requiring approximately 10 hours of computing time.

The simulation reported here advances far beyond what has previouly been reported in the literature as to the size of the simulation system. Such extreme simulation will be feasible for a wider community in the near future as even the pessimistic estimates on the performance development of supercomputers promise significant improvements on the computational capabilities. Bringing the pore-scale simulations to totally new sample sizes (while keeping the resolution fixed) would allow at least a partial bridging of the scales between the length scales that can be reached within pore-scale simulations and continuum models or experiments.