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A prospect for computing in porous materials research: Very large fluid flow simulations

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ABSTRACT

Properties of porous materials, abundant both in nature and industry, have broad influences on societies via, e.g. oil recovery, erosion, and propagation of pollutants. The internal structure of many porous materials involves multiple scales which hinders research on the relation between structure and transport properties: typically laboratory experiments cannot distinguish contributions from individual scales while computer simulations cannot capture multiple scales due to limited capabilities. Thus the question arises how large domain sizes can in fact be simulated with modern computers. This question is here addressed using a realistic test case; it is demonstrated that current computing capabilities allow the direct pore-scale simulation of fluid flow in porous materials using system sizes far beyond what has been previously reported. The achieved system sizes allow the closing of some particular scale gaps in, e.g. soil and petroleum rock research. Specifically, a full steady-state fluid flow simulation in a porous material, represented with an unprecedented resolution for the given sample size, is reported: the simulation is executed on a CPU-based supercomputer and the 3D geometry involves $16{,}384^3$ lattice cells (around 590 billion of them are pore sites). Using half of this sample in a benchmark simulation on a GPU-based system, a sustained computational performance of 1.77 PFLOPS is observed. These advances expose new opportunities in porous materials research. The implementation techniques here utilized are standard except for the tailored high-performance data layouts as well as the indirect addressing scheme with a low memory overhead and the truly asynchronous data communication scheme in the case of CPU and GPU code versions, respectively.

1. Introduction

The persistent progress in computational software and hardware offers evermore powerful tools for research and development. The theoretical peak performances of the top supercomputers are currently measured in tens of petaflops [1], and there are already several scientific softwares which reach a sustained performance of even tens of petaflops (see e.g. Refs. [2–9]). However, when it comes to a specific research field, the relevance of this immense computational power to solving outstanding research problems is not immediately clear. We must ask ourselves what kind of research tasks can be tackled by fully harnessing the modern computational resources available, or how we can exploit the resources in a meaningful way, and which in fact the ambitious and realistic research questions from purely a computational point of view are. Here we will consider these aspects in connection with soil research and reservoir evaluation.

1.1. The computational challenge

In structured heterogeneous soils, water and solutes can be largely transported through macropores, and they can thereby bypass most of the pore matrix. This kind of rapid preferential

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flow is an important phenomenon in agricultural soils due to its implications on the fast movement of contaminants through the soil profile both in their dissolved and colloid-bound forms [10]. Since macropores are relatively sparsely distributed in soils, quite large soil samples would be necessary in imaging so as to capture a representative volume element (RVE). In order to have a representative sample, typical soil cores used in experiments are ca. 20 cm in diameter. At the same time, pores larger than 100 μm have been found to participate in the preferential flows.

To reliably include pores of this size in simulations of fluid flow through soil samples using, e.g. the lattice-Boltzmann method [11,12], an image resolution of about 20 μm would be needed. So far the largest reported lattice-Boltzmann simulations in 3D soil images, obtained by X-ray microtomography, have used samples with a voxel count of about 1000^3 (see e.g. Refs. [13,14]). A resolution of 20 μm would have thus allowed the simulation of soil samples with an edge length of 2 cm, which is about ten times smaller than the required size for RVEs. Thus, an order of magnitude increase in the size of the simulation domain would lead to important benefits in this research problem. Obviously such a simulation would still neglect a significant part of the small pores important in many transport processes, but the advance in the state-of-the-art is clear in terms of characterizing the soil macropore networks and studying the preferential and non-equilibrium flows.

Characteristic length scales of an oil reservoir rock, in turn, can vary from kilometers to nanometers depending on the extension of the reservoir and on the size of the smallest rock structures that can contain oil. In case of a conventional siliciclastic reservoir rock, for example, the mean diameter of pore throats is generally more than 2 μm, while in a shale rock these throats can be as small as 5 nm [15]. In carbonate rock, on the other hand, multiple porosity and permeability systems can coexist in a reservoir, both due to the deposition characteristics of the rock and a large variety in the diagenesis processes [16,17]. Diagenesis, i.e. the chemical and physical changes that occur in a reservoir after the deposition of the rock, can strongly modify its properties by creating in the rock different kinds of microporosity or large structures like vugs and caverns. A visualization by very high resolution X-ray microtomography of carbonate rock is shown in Fig. 1.

Several tools are used to characterize reservoirs: the acquisition of seismic data can cover an area of many square kilometers with a resolution of a few tens of meters, various logging tools are used after the drilling process to characterize the rock at or near the surface of a well with a resolution limited to a few tens of centimeters, and, finally, the rock obtained during the drilling process (i.e. drilling cores, side-wall samples, and/or cuttings) can be investigated in greater detail. The dilemma of course is that, in general, rock properties can be measured with good accuracy from small samples, but, at the same time, the correlation of the observed properties with those of the rest of the reservoir is degraded. Hence, the most important task in everyday reservoir evaluation is to properly up-scale the properties measured at a small scale.

The most commonly used sample for direct, or indirect, laboratory measurements of rock properties before any up-scaling processes is a plug. Plugs are extracted from core samples recovered during drilling, and typically they have a diameter of 3.8 cm and are 5–10 cm long. In the current state-of-the-art digital-rock physics [8,19,20], samples of conventional reservoirs with the average pore throat of the order of 2 μm, which thus determines the maximum voxel size, are simulated using a mesh of 2000^3 voxels corresponding to an edge length of 4 mm in the sample. Ten times larger simulation domains are hence required to reach sizes which correspond to the diameter of a plug. Such an advance in the computational capacity would not only increase the representativeness of the simulated properties, but would also help to improve their up-scaling from the plug scale to a whole-core scale.

1.2. A response to the challenge: aims and means

To summarize, porous materials with complex internal structures, typically involving multiple scales, present serious challenges to computational materials research. In the case of soil research, very large simulation domains are called for in order to reliably capture transport properties of RVEs. In reservoir evaluation the general dilemma is similar: rock properties can be measured accurately for small samples, but then the correlation of the observed properties with those of the rest of the reservoir is compromised. Thus, a fundamental task in everyday reservoir evaluation is to properly up-scale the properties measured at a small scale.

An increase in the size of pore-scale flow simulation domains by an order of magnitude would lead to significant progress both in soil and reservoir rock research. First of all, such *ab initio* simulations can improve our understanding of the fundamental relation between structure and transport properties in heterogeneous materials. Secondly, this progress would benefit more complex multiscale-modeling approaches where the larger scale continuum models require input from the pore scale simulations [21,22]. For example, the so-called heterogeneous multiscale methods use a general macroscopic model at the system level while the missing constitutive relations and model parameters are locally obtained by solving a more detailed microscopic model [23,24]. At large enough scales, however, the low resolution and the lack of available data often necessitate rough descriptions of governing processes and parametrizations based on a simplified picture of the pore structure. Therefore, if pore scale modeling would be able to capture the heterogeneity of the porous medium up to the size of RVE, the utilization of advanced multiscale-modeling techniques would become more viable and reliable tools in solving practical problems related to multiscale porous materials including up-scaling transport properties from, e.g. the plug scale to a whole-core scale.

Here we demonstrate that current computing capabilities already allow a direct pore scale simulation of transport phenomena in porous materials using system sizes far beyond what has previously been reported in the literature. The achieved system sizes readily close the particular scale gaps discussed above. In this demonstration, we simulate fluid flow through a very large sandstone sample using the lattice-Boltzmann method. The simulated flow field provides the average flow velocity through the sample which, in turn, allows determination of the sample permeability. In order to better demonstrate the current computing capabilities in porous materials research, we execute simulations with two separate implementations, i.e. with CPU and GPU code versions. The implementation techniques utilized are standard except for the tailored high-performance data layouts as well as the indirect addressing scheme with a low memory overhead and the truly asynchronous data communication scheme in the case of CPU and GPU code versions, respectively. In our case study we utilize synthetic X-ray tomography images representing microstructure of Fontainebleau sandstone.

We begin by presenting the lattice Boltzmann method together with technical details concerning data layouts and memory addressing schemes in Section 2. Section 3 covers in detail the properties of the porous samples of Fontainebleau sandstone. Section 4 explains the main weak and strong scaling results from simulations on CPU- and GPU-systems. Results from the fluid flow simulations, i.e. the computed permeability values, are also explained in