Nanoporous Flow Simulations on the Summit Supercomputer

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ABSTRACT

Fluid flow behaviors in nanoporous materials can be distinct from those following the continuum physics at higher scales. Numerical simulations can be a complement to laboratory experiments. This work presents a dissipative particle dynamics (DPD) package for GPU-accelerated mesoscale flow simulations in nanoporous materials. In an ideal benchmark that minimizes load imbalance, the package delivered nearly perfect strong- and weak-scaling (with up to 4 billion DPD particles) on up to 1,536 V100 GPUs on Oak Ridge National Laboratory's Summit supercomputer. More remarkably, in a benchmark to measure its usefulness with realistic nanopores in SBA-15 silica, the package exhibited more than 20x speedup over its LAMMPS-based CPU counterpart with the same number nodes (e.g., 384 V100 GPUs vs. 2,688 POWER9 cores). It is also worth highlighting that the NVLink2 Host-to-Device interconnects kept the cost of CPU-GPU memory copy as low as only 10% of GPU activity time per rank, which is 4 times less than their PCIe counterparts.

KEYWORDS

Summit supercomputer, GPU computing, nanoporous materials, dissipative particle dynamics

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1 INTRODUCTION

In geosciences, the permeability of natural nanoporous materials such as kerogen-rich tight shale is difficult to characterize, because of their highly non-uniform distribution of pores, because of their heterogeneity of material properties that can impact the fluid inside physically and chemically, and because of the limited capacity of laboratory instrumentation. It is hard to agree on a common approach to study flow and transport phenomena in natural nanoporous materials, as too many coupled variables should be considered.

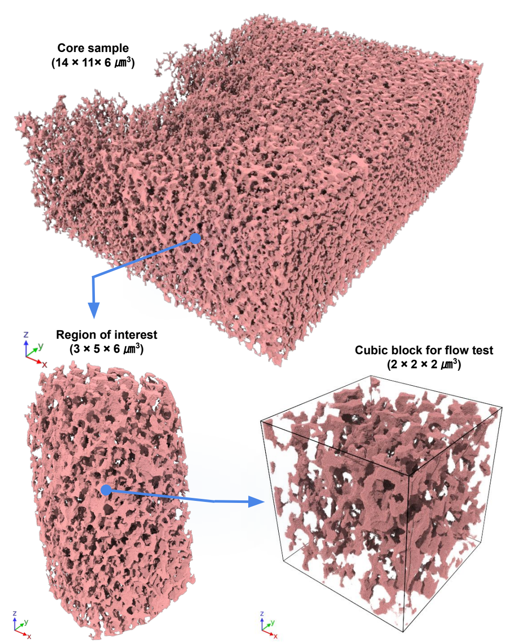

Figure 1: Pore skeleton of a SBA-15 silica sample obtained by FIB-SEM (focused ion beam scanning electron microscope) with voxel resolution of 7.7^3 nm^3 (top). A region of interested (ROI) extracted for fluid-permeability analysis (bottom left). A cubic block extracted from the ROI for DPD flow simulations (bottom right).

Synthetic mesoporous silica are often used for studying fluid flow and transport at the nanoscale, as they are architected with controlled material properties, pore sizes and distributions. This work uses SBA-15 silica as the nanoporous media to measure water-permeability dependence. Selection of a proper computational domain is illustrated in Figure 1. Over 100 million DPD particles are

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required to run for an equivalent number of timesteps for measurement. A simulation code that is able to take full advantage of the latest supercomputers is critical to the success of the study.

2 APPROACH

This work employs userMESO 2.5 [6] — the latest release to the userMESO framework developed as a GPU extension package to LAMMPS [4] for DPD simulations [1, 5]. New features mainly include implementation of the many-body DPD model [3, 7] and an impenetrable wall boundary model for arbitrary geometries [2]. Notable innovative features of the package are discussed in [5]. In userMESO, all computations and host-device communications are handled by the extension package, while I/O related tasks such as inter-rank communications are attended by LAMMPS. All releases of userMESO (i.e. version 1.0, 2.0 and 2.5) are able to achieve excellent strong- and weak-scaling on ORNL's Titan supercomputer as well as competitive speedup over its CPU counterpart [1, 5, 6].

3 RESULTS

Code readiness on Summit has been made for userMESO 2.5. Like most people did to show scalability using a benchmark with minimal load imbalance, we used a manufactured, strictly uniform pore system, with which userMESO 2.5 delivered nearly perfect strong- and weak-scaling (with up to 4 billion DPD particles) on up to 1,536 V100 GPUs on Summit (6 GPUs and 42 usable Power9 CPU core per node); see Figure 2. To measure how userMESO 2.5 performs

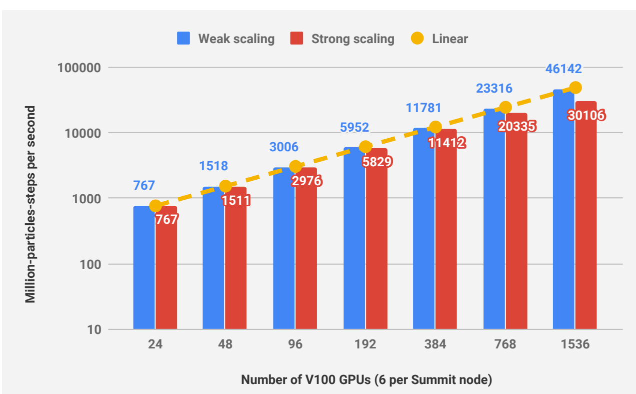

Figure 2: Strong- and weak-scaling performance on Summit.

for non-uniform pores, strong-scaling was conducted with a cubic block SBA-15 silica geometry as shown in Figure 1 (about 70 million DPD particles), exhibiting more than 20x speedup over its CPU counterpart with the same number nodes (e.g., 384 GPUs vs. 2,688 CPU cores); see Figure 3. A maximum load imbalance factor of 2.9 is observed. This indicates that GPU computing, with fewer partitions, effectively reduces load imbalance than its CPU counterpart. Moreover, a breakdown of rank-averaged GPU activity time is displayed in Figure 4, showing a low ratio of time cost of host-device memory copy thanks to the NVLink2 Host-to-Device interconnects. Note that it is 4 times less than their PCIe counterparts on DGX-1 and half of the cost than NVLink1 on SummitDev.

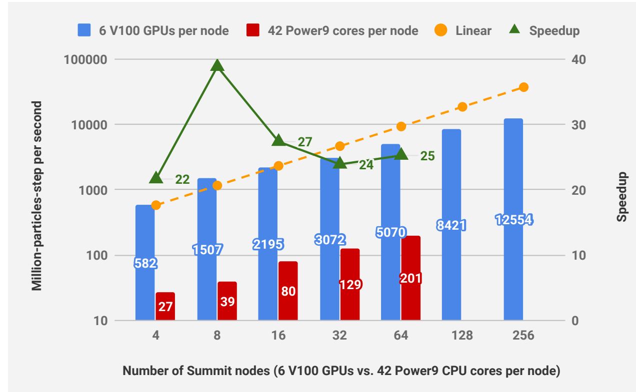

Figure 3: GPUs vs. CPUs with the same nodes on Summit.

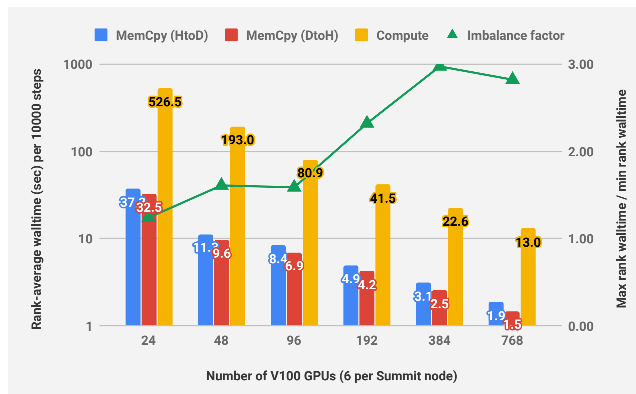

Figure 4: Breakdown of GPU activity time on Summit.

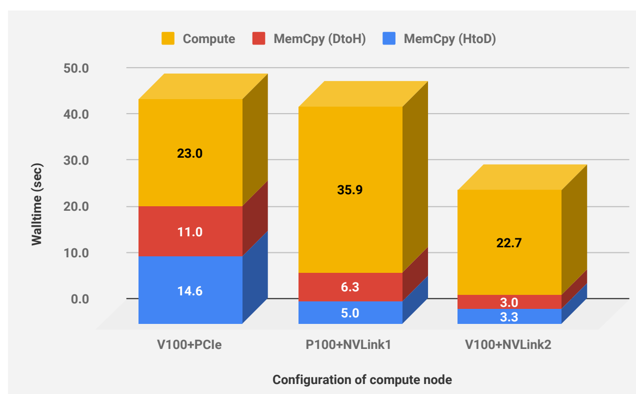

Figure 5: Single-node breakdown of GPU activity time.

Above all, our study has demonstrated the success of userMESO 2.5 and DPD methods on Summit. A broader implication is that other particle-based methods such as smoothed particle hydrodynamics (SPH) and discrete element method (DEM) may also benefit tremendously from the dense GPU configuration and the overall GPU-computing power provided by Summit.

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