The Computational Kernel

This GISAXS scattering pattern simulation code is based on the Distorted Wave Born Approximation (DWA/B) theory, and involves a large number of computer-intensive form-factor calculations. A form-factor at a given point in the inverse space is computed as an integral over the shape volume functions of the nanoparticles in a given sample. By applying Green’s theorem, this volume integral can be transformed into a surface integral over the shape boundary. The scattered light intensity at a point is proportional to form-factors at that point. A simulated sample structure is taken as an input in the form of discretized structure surfaces, such as a triangulated surface. For our computational purposes, form-factor is described as a summation over the discretized surface of the shapes under consideration. Such form-factors are computed for all points in a inverse space grid, the $q$ grid.

Parallelism Hierarchy

The $q$ grid (in inverse space) is decomposed into tiles, each assigned to a different processor. It is further divided into hyperblocks along with triangles, each computed one at a time on the device. This helps to hide host-device transfer latency. A hyperblock is decomposed into thread blocks. During computation within a thread block, input triangles data is loaded into the shared memory, and all threads access each triangle to compute the form-factors.

Multiple such computations may be executed in a single run, each with different experimental configuration. Each configuration is executed in parallel, and this becomes the highest parallelism level in the hierarchy.

Performance on Single and Multiple GPUs

Performance of GISAXS on the Cray Xk7 Titan supercomputer (with a K20X GPU per node) compared with Cray XE6 Hopper supercomputer (with dual AMD Magny Cours, 24 cores, per node) and Cray XC30 Edison supercomputer (with dual Intel Sandy Bridge, 16 cores, per node) are shown below.

Conclusions

GISAXS is enabling fast X-ray scattering simulations and data analysis using parallel computing. GPU powered systems prove to be ideal platform for computations in GISAXS. It is able to achieve 1 Petaflops using 8192 nodes on Titan (Cray Xk7). For comparison, it achieves 0.63 Petaflops using 14400 cores on Hopper (Cray XE6), 0.2 Petaflops running 8192 cores on Edison (Cray XC30), and 0.6 Petaflops using 1024 nodes on Stampede (Intelllic M/C cluster).

We also note that GPUs proved to be the most energy efficient as well with a performance per watt of 9 GFlops/W on Nvidia K20X GPU, compared to just 1.3 GFlops/W on AMD Magny Cours, 3.3 GFlops/W on Intel Sandy Bridge processors, and 2 GFlops/W on an Intel M/C co-processor.

Acknowledgements

This work was supported by the Director, Office of Science, U.S. Department of Energy (DOE) under contract no. DE-AC02-05CH11231. This research used resources of the National Energy Research Scientific Computing Center (NERSC), which is supported by the Office of Science, U.S. DOE, under contract DE-AC02-05CH11231, and of the Oak Ridge Leadership Computing Facility (OLCF), which is supported by the Office of Science, U.S. DOE, under contract no. DE-AC05-00OR22725. The authors also acknowledge the Texas Advanced Computing Center (TACC) for providing GPU resources that have contributed towards the reported results.

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