Large-scale Particle Simulations using Dynamic Load Balance on TSUBAME 2.0 Supercomputer

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We have developed a simulation code of the Distinct Element Method (DEM) for multi-GPU computing. Domain decomposition is a reasonable way to achieve high efficiency for parallel computing on the machines with multiple nodes. However, the particle distribution changes in time and the computational load for each domain gradually becomes quite non-equal.

In this study, we introduce an effective method to realize the dynamic load balance of a particle simulation on a GPU supercomputer. By applying the slice-grid method, we maintain the same number of particles in each domain. Several techniques for particle counting and data movement are implemented. The time integration causes memory fragmentation and the frequency of the memory de-fragmentation on CPU is examined accounting for the cost of the data communication between CPU and GPU to recover the computational performance. A link-list technique of the interaction particle list is introduced to save the memory drastically.

Our dynamic load balance works well with good scalability in the number of GPUs. A banker-shot simulation of golf player is demonstrated with over 50 million particles using 512 GPUs on TSUBAME 2.0 of Tokyo Tech.

Keywords: Distinct Element Method, multi-GPU computing, Dynamic load balance