Towards Multicolor Particle Contact Detection Method for Hybrid MPI-OpenMP Execution in DEM

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Abstract. We evaluate a parallel implementation method for particle contact detection processes in the Discrete Element Method (DEM). By using multicolor contact grids, our implementation method, called the Multicolor Particle Contact Detection Method (MPCD), accomplishes parallel execution without mutual exclusion. The MPCD is well-suited for hybrid MPI-OpenMP execution. In addition, there is possibility to improve load imbalance if we use "particle parallelism" for computations in node in case of MPI execution.

Keywords: Large-scale Simulations in CS&E, Parallel and Distributed Computing

1 Introduction

Discrete Element Method (DEM) is a numerical method that is frequently utilized in various kinds of scientific and engineering computing fields, such as materials design. In the DEM, all particles have a chance to make contact with other particles. Our objective is to speed up contact detection and ensuing processes (which we henceforth call *particle contact detection (PCD) processes*). We evaluate a new parallel implementation method for PCD processes that utilizes multicolor grids to actualize parallelism among the PCD processes, which is called *Multicolor Particle Contact Detection Method (MPCD)*.

The Spatial Decomposition Coloring (SDC) [1] was proposed for Molecular Dynamics (MD). The SDC is the same concept as MPCD in viewpoint of using multicolor grid to obtain high efficiency for OpenMP. The following difference can be pointed out for the MPCD: (1) The target is DEM, (2) With respect to computations in hybrid MPI-

OpenMP execution, and (3) There is possibility to improve load imbalance in node by utilizing "particle parallelism" [2] in MPI execution.

3 Preliminary Performance Evaluation

We used the Fujitsu FX10 supercomputer system (FX10) installed at the University of Tokyo to conduct performance evaluations The CPU architecture of the FX10 is SPARC64 IXfx (1.848 GHz), with 16 cores per node, and theoretical peak performance per node of 236.5 Gflops. The main memory per node is 32 GB, and the aggregate bandwidth for memory per node is 85 GB/s. We used the Fujitsu Fortran90 compiler version 1.2.1 P-id: T01641-02 with compiler option "-Kfast, openmp." In sequential execution (#threads=1), we did not use OpenMP compilation. We also specified inline option for the kernels of the PCD processes.

We solved a 3D DEM problem with gravity. We only computed the forces on each particle for the horizontal direction. The initial locations of the particles were set with random numbers as [0, 1], [0, 1], [0, 1]. We used 62,499,988 particles in the experiment. Particle diameter, particle density, spring constant between two contact particles, and restitution coefficient were set to 2.000E-03, 1.000E+03, 1.000E+02, and 8.000E-01, respectively. The time interval (dt) of the simulation was 1.2860E-04. Fig. 1 shows the average execution time for the three methods.

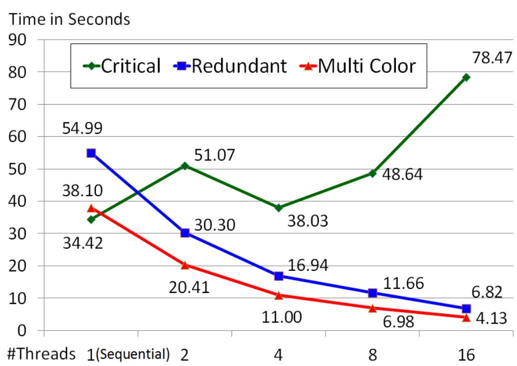

Fig. 1. Execution time for each method for average time step. Maximum time step of 20 and accumulated the execution time from fourth step to the twentieth step is shown. "Critical" is a conventional implementation with a mutual exclusion. "Redundant" is a conventional implementation with double of computations, but no mutual execution. "Multi Color" is the method to use MPCD.

Fig. 1 shows the MPCD ("Multi Color") is superior to other two conventional implementations. The performance results with Hybrid MPI-OpenMP execution will be presented in the poster session.

References

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