

# Large Scale MPI-Parallelization of LBM and DEM Systems: Accelerating Research by Using HPC

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**Abstract**—Casting, solidification, and the behavior of dry, saturated, and partially saturated granular media are examples of interesting and important problems in multiple areas of civil, mechanical, and chemical engineering. For interacting particle-fluid systems, the Discrete Element Method (DEM) and Lattice-Boltzmann Method (LBM) provide valuable high-resolution numerical models. Their main issue is high computational demand, which can be addressed by use of HPC resources. This work demonstrates the use of MPI-parallelized LBM and DEM models to accelerate research in solidification and macroscopic behavior of dry and saturated granular media. Large scale parallel simulations of dendritic growth, the calibration-chamber cone penetration test, and a parametric study of shear thickening in granular suspension were performed. Use of HPC dramatically reduced the computational time for these studies and provided high-resolution representation of physical experiments.

**Index Terms**—lattice-Boltzmann method, discrete element method, parallel, MPI, HPC

## I. INTRODUCTION

The principal limitation of DEM is the large computing requirements for practical problems. DEM was recognized nearly two decades ago as a viable alternative to continuum methods for modeling of granular media [1]–[4]. At that time, the computing capabilities and the understanding of granular physics put the method at the boundary between academic investigations and practical applications. During this time period, Cundall [5] suggested 20 years would be needed to make discrete element methods viable for practical engineering analysis.

In the time since, both the computer hardware and the basic understanding of the granular mechanics [6] underlying the method has brought DEM into the realm of practical analysis [7]–[9]. This assessment is certainly valid for many applications that can be solved for particles counts of  $10^6$

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or less. Materials handling applications and basic granular media research dominate such problems [10]–[12]. However, computer technology now makes simulations with particle counts in the range  $10^7 - 10^8$  possible [13]. Recent work [14] shows feasibility of 2.4 billion particle calculation in real scale.

Large scale LBM systems [15] were developed comprising hundreds of billions of nodes each holding multiple distribution functions. They are especially suitable for applications involving fluid flow, diffusion, and heat transfer within complex boundaries. Our LBM development focused on large-scale solidification modeling applications [16]–[19] and coupled DEM+LBM micromechanical modeling of shear thickening [20], [21].

## II. DEM PARALLELIZATION SCHEMES

The use of parallel computing with DEM was described for terramechanics problems by [2]–[4]. These early efforts at parallelization of particles in a box were based on a simple domain decomposition in which particles were assigned to processors based on their position in a two dimensional Cartesian grid. The scheme was simple, with easily defined processor communication patterns. But the method did not efficiently address many of the complicated problems in a

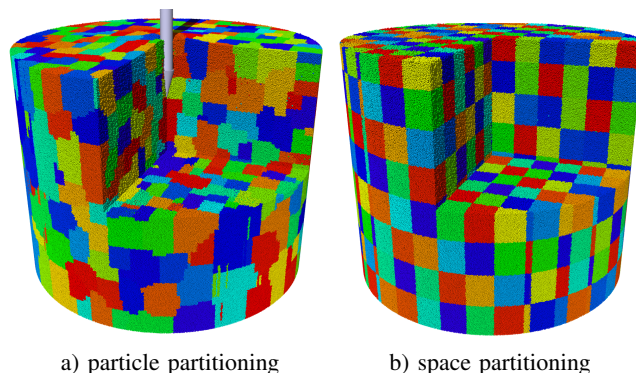


Fig. 1. Processor assignments.

more general setting including complex domain shapes, load imbalance, and elongated shapes. The approach gave limited partitioning options, and those available were often ill-suited for irregular domains or large processor counts.

The approach taken in the present work seeks to eliminate the load balance problem and the particle size and shape restrictions through the use of a more subtle parallelization design. The new approach no longer ties *space* to a processor; rather, the particles are initially assigned to processors based on a chosen criteria, with the assignment remaining throughout the computation. A preferred choice for the processor assignment criteria is locality of particles, which can take advantage of the knowledge of initial geometry. This method not only allows the partitioning to be performed outside of the DEM model, but also allows the partitioning to take a far more complicated form if necessary. In the present implementation, the particle ownership is static, meaning it does not change as particles move, which decreases data movement among processors. Then, a “processor space” is defined by a gridded subdivision of the simulation domain which creates a cell structure that is common on all processors. Particles are assigned to this space according to their evolving locations. A processor’s ghost particles are determined by finding those particles on other processors that share similar processor space. After the ghost particles are received from other MPI processes, the neighbor search is performed locally using the bounding box method [22]. A major drawback to this approach is that the ghost particle determination is far more computationally intense, and the processor communication patterns are constantly changing. The method also requires an all-to-all processor communication to compare shared “processor space”, which becomes more of a computational burden as processor counts increase. However, the use of an “expanded” particle radius during the ghost particle determination helps reduce the computation cost of this technique. Using the expanded radius reduces the costly list update requirement to only when total movement of any particle exceeds the expanded particle radius size, which usually requires many time steps. Although the expanded size increases the number of ghost particles on each processor, the larger particle counts are far less computationally expensive.

Finally, the method requires effective partitioning strategy because poor particle partitioning can result in excessive memory use. Since the partitioning is performed independent of the simulation, a user can use any method they choose. Simple partitioning such as the columns mentioned earlier can be used when appropriate, or more complicated tools such as ParMETIS [23] can be employed. The ParMETIS algorithm distributes particles to optimize some specified criteria, such as uniform distribution or minimized communication between processors. When more complex particle domains with non-uniform particle density need to be distributed between processors, particle partitioning with ParMETIS tool eliminates user intervention and guarantees satisfactory load balance.

### III. PARALLEL PERFORMANCE

Initial lid-compaction phase for a 9.5 million particle configuration settled in a rigid cylindrical mold, as shown in Figure 1 a), was chosen as a benchmark to measure parallel performance.

The present particle partitioning technique was then compared with the space partitioning (Figure 1 b)) as implemented in open-source LIGGGHTS DEM package [24]. The benchmark examined settling of 9.5 million particles under gravity.

Starting configuration for the LBM speedup measurement is shown in Figure 2. Further details of parallel LBM solidification model are described in references [16]–[19]. Our work on DEM+LBM coupling, where the LBM system is executed in parallel and DEM is serial (duplicated among the MPI processes), is presented in [20], [21].

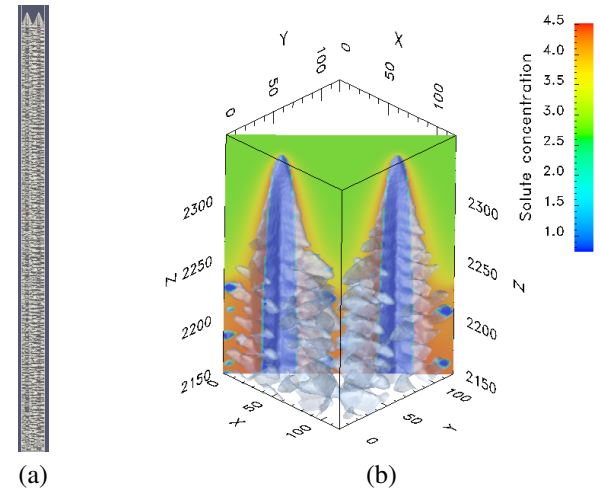


Fig. 2. (a) Starting configuration for LBM speedup test. (b) Zoomed-in portion at the top of dendrites, showing wt.% of solute.

Speedup plots for A) DEM with particle partitioning, B) DEM with space partitioning, and C) LBM solidification model with spatial domain decomposition are shown in Appendix A. DEM particle partitioning performs better at low number of MPI processes, while DEM spatial partitioning is advantageous for large number of MPI processes.

### IV. CONCLUSIONS

Significant speedup can be achieved in many numerical solvers with real-world engineering applications. Although DEM and LBM have become mature tools for micromechanical investigations into the science of granular media, their use in macroscale analysis is still in its infancy. The macroscale success of these methods depends on the availability of sufficient computing resources to make their use practical. This work demonstrates that modern parallel computing provides the resources to make DEM and LBM effective tools for problems once beyond the capabilities for numerical analysis. If computing resources continue to grow and become more generally available, DEM and LBM will become increasingly attractive engineering tools.

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