A MPI/domain decomposition strategy for large-scale simulations of granular media made of particles of arbitrary shape

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ABSTRACT

In [1] we suggested a novel variant of Discrete Element Method (DEM) to simulate systems of granular media made of arbitrary non-spherical convex particles. This formulation is now extended to parallel computing by using a domain decomposition method and Message Passing Interface (MPI) for sub-domain communications. Our code Grains3D is a CPU-based DEM code [2,3,4] well suited to multi-CPU architecture and implemented in C++, a flexible, high-level programming and object-oriented language. Due to modern multi-core architecture, we adopt a programming strategy that optimizes memory management as well as a domain decomposition communication pattern that minimizes the communication overhead. In systems which exhibit decent load balancing, we quantify the impact of our programming strategy on the performances of Grains3D. We illustrate satisfactory scalability of Grains3D on parallel simulations of systems such as a silo discharge [5], a rotating drum [6] and a granular slumping [7] with up to a hundred million of both spherical and non-spherical particles.

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