Abstract

Large-scale industrial simulations of bulk solids using the Discrete Element Method (DEM) involve enormously large number of particles. Although DEM seems to be well established, it becomes problematic when the number of particles is very high and the simulation needs to be done on a single personal computer within a limited time period. Therefore, coarse-graining appears to be an effective technique for reducing the computational demands for such scenarios. The main theme of the thesis is to introduce coarse-grained particles efficiently and dynamically in DEM simulations to reduce the simulation time while maintaining the accuracy of the output.

Most of the current coarse-graining techniques use a uniform coarse-grain ratio throughout the equipment. Such uniform coarse-graining severely limits the degree of coarse-graining possible because, at the higher coarse-grain ratio, the accuracy of the simulation can be affected. To resolve this issue, a multi-level coarse-graining technique (MCG) has recently been proposed by Queteschiner *et al.* [1] where the coarse-grain ratio varies spatially. In this work, we propose a simpler particle location-based method for multi-level coarse-graining. The new method can be readily implemented using open-source software LIGGGHTS Public (DCS Computing GmbH, Linz, Austria). In this method, the coarse-grained particles disintegrate into particles of higher resolution in the refinement step at the desired spatial location, and the opposite occurs during the coarsening step. The efficiency of this new coarse-graining method has been demonstrated successfully using discharge from a conical hopper as an example. Compared to uniform coarse-graining, the computational time is reduced by more than an order of magnitude without compromising on accuracy.

Our new multilevel coarse-graining method (MCG) [2] has been demonstrated for a hopper-screw feeder system as well in this work. In contrast to the conical hopper system, the hopper-screw feeder system is characterized by complicated flow patterns, moving geometry, rapid movement, and recirculation. Despite these complexities, the proposed MCG technique could capture the critical features of the powder flow for this system and reduce the computation substantially. A few key factors hitherto neglected in the literature, such as meshing and processor mapping, are also explored thoroughly. It is also observed that accounting for the moving part of the mesh consumes significant computation time and reduces the degree of speed-up achieved by MCG. It has also been shown that the proposed MCG technique has a much higher potential than what appears prima facie.

In industries, often a small amount of liquid is added to dry powder-like particles to introduce cohesive nature in the particles of the system. Any such process with wet particles can be simulated with DEM. Capillary force and viscous force are taken into consideration to simulate such a system, including wet particles using DEM. In this thesis, we have proposed the scaling laws of surface tension and viscosity of liquid when we use coarse-grained wet particles. It is shown that surface tension and viscosity are to be scaled by l for coarse-grained particles where l is the coarse-grained ratio (ratio of diameters of coarse-grained and original particles).

The proposed model is evaluated by simulating mixing phenomena. The velocity distribution and Lacey's mixing index of the coarse-grained simulations are in good agreement with the simulation taking resolved particles.

DEM simulates granular processes and detects inter-particle collisions during the simulation. Detection of collision helps researchers to study the occurrence of particulate mechanisms such as aggregation, breakage, etc. The frequency and probability of collisions for different particle size classes may change when coarser particles are introduced. This thesis introduces a new mathematical formulation, namely the collision dependency function (CDF), which predicts the probability of collisions between different particle classes for systems containing resolved and coarse-grained particles. The CDF is extracted by executing one DEM simulation consisting of number-based uniformly distributed particles. Furthermore, a new optimized scheme is used inside the DEM to store the collision data efficiently. Finally, the collision probabilities between size classes obtained from DEM simulations are compared successfully against their counterparts calculated from the developed model for verification.

One of the promising approaches to characterize the evolution of the mesoscale features of the particulate process is the population balance model (PBM). The PBM-DEM coupled framework can simulate the particulate processes such as aggregation and breakage etc. The DEM simulations consume the most computational cost in PBM-DEM coupled framework. This thesis introduces CG particles in a PBM-DEM coupled framework using a novel technique. The resolved simulation coupling framework is based on earlier work of [3]. In this framework, PBM receives the collision frequency and particle count from the DEM simulation, and PBM then solves the governing equation to produce the updated particle size distribution (PSD). Due to the lower particle number density in the CG system, fewer collisions occur than in the resolved system. A new scaling law has been developed to determine the collision frequency of the resolved system from the CG system. Two test cases have been used to validate the new scaling rule. Accordingly, the entire PBM-DEM coupled framework has been revised for CG particles. The resolved simulation and CG simulation have successfully been compared in terms of simulation time and other findings.

References

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