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Multi-level coarse-grain model of the DEM

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ABSTRACT

The ability to model granular systems at the level of individual particles has largely conduced to the success of the discrete element method (DEM). At the same time, this fundamental concept hinders the use of the DEM for industrial-scale simulations as the computational cost of the method increases with the size of the system. The DEM coarse-grain (CG) model provides one means of counteracting this effect by replacing a group of original particles by a larger (pseudo) particle. The major shortcoming of this approach is that it fails to capture effects that intrinsically depend on particle size. To overcome this deficiency we have devised a novel model to efficiently combine multiple levels of coarse-graining in a single DEM simulation. While a coarse realization is used where it sufficiently represents the granular flow, the level of resolution may be increased recursively in spatially confined regions of interest. Thus, the method is able to benefit from the speedup of the coarse-grain approach and retain the details of the granular system in crucial regions. Two-way coupling between different levels of resolution is established by passing volume-averaged flow properties. We present validation data based on the comparison between the computed statistical properties of our multi-level coarse-grain (MLCG) model and the corresponding properties of the fully resolved reference system.

1. Introduction

Since its introduction by Cundall and Strack in 1979 [1], the DEM has proven to be a valuable tool for the analysis of granular flows. Fostered by the steadily growing computational power, the DEM was able to leave the field of pure academic research and find its way into numerous branches of industry, where it is used to optimize processes and equipment in terms of efficiency, throughput and quality. This applies to such diverse areas as the food [2, 3], pharmaceutical [4, 5] and mining [6] industries, as well as the iron and steel making industry [7]. Major reviews of substantive applications of the DEM are published periodically [8, 9, 10, 11].

Despite the advances in computer hardware and software parallelization techniques such as MPI and OpenMP [12, 13, 14], simulations of industrial-scale problems involving billions of particles easily exceed the limits of feasibility. The demand for ever more detailed physical models in combination with complex industrial geometries aggravates the problem even further, limiting the accessible simulation times and length scales. Still, simulations are an indispensable tool in process analysis, especially in cases, where experimental data is also difficult to obtain. However, to be able to handle the immense amount of particles in engineering-scale problems, it is necessary to cut back on the level of detail and accuracy. A conventional approach is the usage of continuum mechanics in the form of the finite element method (FEM) [15, 16] or the finite volume method (FVM) [17, 18, 19]. A major downside of these methods, though, is their inapplicability to processes that are dominated by the discontinuous behavior exhibited by granular material.

Another approach to address large-scale granular systems and connect the granular dynamics with macroscopic continuum dynamics is the derivation of Eulerian fields from the discrete system [20, 21, 22]. This coarse-graining formulation is designed to yield fields that satisfy the equations of continuum mechanics and can be used to calibrate and validate Eulerian models.

As a different strategy to recover the granular characteristics and increase the depth of physics, spatial multi-scaling techniques have become a practicable approach. The combination of coarse- and fine-scale representations - in confined regions of interest - tries to balance the accuracy of the simulation with the affordable computational expense. For instance, this strategy has been successfully applied in the form of FEM-DEM coupling [23, 24] and CFD-DEM simulations [25, 26, 27, 28, 29]. The underlying idea of combining multiple scales is indeed a more fundamental concept and probably best known from the field of chemistry and molecular dynamics [30, 31, 32].

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In this spirit, we strive for a spatial multi-scale model that retains the Lagrangian character of the granular flow on all scales. To this end, we draw on the coarse-grain model of the DEM as described in [26, 33, 34, 35, 36, 37] (not to be confused with the aforementioned coarse-graining formulation). This technique can ease the severe computational demands of DEM simulations by grouping a number of equal particles together into a representative CG particle, thus effectively reducing the system size. A dimensional analysis of the governing equations yields a set of scaling rules for this approach. However, for effects that inherently depend on particle size, these scaling rules become invalid and the CG model fails to correctly predict the system behavior. In this situation, our model combines the conventional coarse-scale representation with a more detailed realization that is able to capture the decisive effect properly. The embedded fine-scale simulation is spatially restricted to the critical region, while in the remainder of the system a CG representation is maintained. The different levels of resolution are coupled through the exchange of characteristic, volume-averaged flow properties. The concurrent use of coarse- and fine-scale representations allows to speed up the simulation while resolving essential details of the granular system.

2. Method

2.1. Discrete element method

2.1.1. Contact model

In the Lagrangian approach of the DEM, the trajectory of each particle $i = 1, \ldots, N$ in the system is obtained by solving Newton's equations of motion

$$m_i \ddot{\mathbf{x}}_i = \mathbf{f}_i \tag{1}$$

$$\underline{I}_i \dot{\boldsymbol{\omega}}_i = \mathbf{t}_i \tag{2}$$

where each element is characterized by its mass m_i, position $\mathbf{x}_i$, inertia tensor $\underline{I}_i$, angular velocity $\boldsymbol{\omega}_i$, force $\mathbf{f}_i$, and torque $\mathbf{t}_i$. The forces $\mathbf{f}_i$ include external forces such as the gravitational force $m_i\mathbf{g}$, as well as the normal and tangential forces during a binary collision

$$\mathbf{f}_{n,ij} = k_n \boldsymbol{\delta}_{n,ij} - \gamma_n \dot{\boldsymbol{\delta}}_{n,ij} \tag{3}$$

$$\mathbf{f}_{t,ij} = k_t \boldsymbol{\delta}_{t,ij} - \gamma_t \dot{\boldsymbol{\delta}}_{t,ij} \tag{4}$$

with normal and tangential stiffness coefficients $k_{n,t}$ in the elastic terms, damping coefficients $\gamma_{n,t}$ in the dissipative terms, and overlaps $\delta_{n,t}$. Over the course of a collision event, the tangential spring-length $\boldsymbol{\delta}_t$ is updated using the relative tangential velocity to be then projected onto the tangential plane. In each time step $\boldsymbol{\delta}_t$ is truncated such that

$$f_{t,ij} \leq \mu f_{n,ij} \tag{5}$$

where μ is a Coulomb-like friction coefficient. Applying the Hertzian theory and non-linear damping [38, 39], the stiffness and damping coefficients read

$$\begin{aligned} k_n &= \frac{4}{3} E^* \sqrt{R^* \delta_{n,ij}} \\ \gamma_n &= -\beta \sqrt{5 m^* k_n} \\ k_t &= 8 G^* \sqrt{R^* \delta_{n,ij}} \\ \gamma_t &= -\beta \sqrt{\frac{10}{3} m^* k_t} \\ \beta &= \frac{\ln(e)}{\sqrt{\ln^2(e) + \pi^2}} \end{aligned} \tag{6}$$

where e is the coefficient of restitution and E^*, G^*, R^*, and m^* are the effective Young's modulus, shear modulus, particle radius, and mass, respectively. The coefficient of restitution is defined as the ratio of the relative particle velocity before and after the collision $e = -v(\tau_c)/v(0)$ with collision time τ_c and is a constant input parameter in this model. The definition of the effective parameters can be found, for instance, in [40]. Furthermore, a rolling friction model based on an elastic-plastic spring-dashpot approach is added in the equations of motion [41, 42]. Contacts between particles and walls - represented via triangle meshes - are handled analogously with the mass and the radius of a wall element set to infinity.

2.1.2. Neighbor lists

As a general optimization technique our implementation of the DEM uses a Verlet-list in combination with a linked-cell-list to speed up the search of potential contact partners [43]. The cell-size and cut-off distance used for generating these lists are determined by the largest particle in the simulation. The neighbor-list is rebuilt if a particle has moved more than half the cut-off distance since the last build. Also the insertion of additional particles requires an update of the neighbor lists, thus it is desirable to add particles in batches to keep insertion events to a minimum.

2.2. Coarse-grain model

In this study, we follow the coarse-graining approach outlined in [34, 35, 44] whereby a number of equal particles is represented by an upscaled (pseudo) particle. To retain the physical behavior of the original system, the interaction forces have to be adjusted accordingly. This scaling is based on consistent energy density and energy density evolution in the original and coarse-scale system. Clearly, for a uniform effect of gravity, particle density ρ must not change and to conserve kinetic energy, particle velocities must be preserved.

Under these assumptions, a dimensional analysis of Eqs. (3, 4) yields the following invariant parameters:

$$\Pi_1 = \frac{R_j}{R_i}, \Pi_2 = \frac{k_{n,t}}{R_i E^*}, \Pi_3 = \frac{\gamma_{n,t}}{R_i^2 \sqrt{\rho E^*}} \tag{7}$$

Π_1 is related to geometric similarity and means that all particles need to be scaled with the same constant coarse-grain ratio $\alpha = R_{i,CG}/R_i$. A straightforward way to derive at this conclusion is by inspecting the effective particle radius

$$R^* = \frac{R_i R_j}{R_i + R_j} = \frac{R_i \frac{R_j}{R_i}}{1 + \frac{R_j}{R_i}} \tag{8}$$

which needs to scale with α just as R_i. Similarly, when looking at the effective mass

$$m^* = \frac{m_i m_j}{m_i + m_j} = \frac{4\pi}{3} \frac{\rho_i R_i^3 \frac{\rho_j R_j^3}{\rho_i R_i^3}}{1 + \frac{\rho_j R_j^3}{\rho_i R_i^3}} \tag{9}$$

we can note down that $m^* \propto \alpha^3$ since ρ is assumed to remain constant. To obtain Π_2 and Π_3, we substitute the dimensionless mass $m^{*\prime} = m^*/\rho R_i^3$, overlap $\delta_n' = \delta_n/R_i$, velocity $\dot{\delta}_n' = \delta_n/v_0$ and acceleration $\ddot{\delta}_n' = \ddot{\delta}_n R_i/v_0^2$ with the reference velocity $v_0 = \sqrt{E^*/\rho}$ into Eq. (3) and arrive at

$$m^{*\prime} \ddot{\delta}_n' = \frac{k_n \delta_n'}{R_i E^*} - \frac{\gamma_n \dot{\delta}_n'}{R_i^2 \sqrt{\rho E^*}}. \tag{10}$$