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Coarse Graining for Large-Scale DEM Simulations of Particle Flow – An Investigation on Contact and Cohesion Models

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Abstract

In this paper we follow the work of [7] to evaluate the scalability of contact law for a linear spring dashpot (LSD) model. Models are evaluated using a shear test box with Lees-Edwards boundary conditions. Afterwards we extend our analysis for a Hertz model and a limited analysis in cohesive contact model. Results demonstrate that Hertz model has the same behaviour as the scaled LSD model for both inertial and quasi static regime. In coarse graining we expect constant stresses values for different parcels sizes. Both models demonstrate an almost constant stress in the quasi-static regime, but a significant increase is obtained in the inertial regime. A limited number of analysis were also made for a JKR cohesive contact model.

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1. Introduction

Discrete element modeling is a numerical method that simulates particle dynamics based on individual particle collisions. Therefore computational effort increases with the increase of the number of particles simulated, which may result in prohibitive computational times when simulations of more than 10 million particles are necessary.

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However, many industrial sectors like powder metallurgy, minerals processing, iron- and steelmaking, chemical industry and many more run processes containing huge amounts of powder or particles in their processes. Die filling process for example in powder metallurgy deals with a prohibitive number of particles to be simulated in most of the cases. Coarse graining allows reducing the computational effort by replacing individual particles by representative parcels, substantially reducing the required number of particles to represent a process. However analytical considerations and verifications are necessary to ensure that the physics is captured correctly.

1.1. Model Description

Discrete element method (DEM) was first developed by [4]. The method aim at tracking individual particles or parcels representing a number of particles in the flow domain. Particles interactions are modelled using a soft-sphere model where rigid spheres are allowed to overlap each other at the contact point.

Giving the sum of forces f_i total force due to contacts with other particles or walls acting on particle i, the changes in positions and velocities of the particles are calculated from the integration of Newton's equation of motion. For translational motion of particle i the equation is given as [6]:

$$m_i \frac{d^2}{dt^2} r_i = f_i + m_i g \quad , \tag{1}$$

where m_i is the mass of the particle i, r_i is the position of particle i and g is the gravitational force. Also for the rotational motion of the particle i the equation is given as [6]:

$$I_i \frac{d}{dt} \omega_i = t_i \, , \tag{2}$$

where I_i is the moment of inertia of particle i, ω_i is the angular velocity of particle i and t_i is the total torque on particle i.

1.2. Normal contact force law

To perform correct simulations using coarse particles one has to think on how to connect the original particle interaction parameters with the coarse particle parameters. Spring and stiffness parameters must be scaled when particle size is scaled.

Following the work of [7], the analysis is based on equal energy densities in the original and the coarse grained system. The density of the particles and the translational velocity must be invariant. Also, the total rotational kinetic energy of the original and coarse grained system must be the same.

The following analysis is valid for a linear spring-dashpot model with frictional slider. We start looking at the differential equation for the normal overlap based on Newton's equation of motion [7]:

$$m_{eff} \ddot{\delta}_n = k_n \delta_n + c_n \dot{\delta}_n \tag{3}$$

Here the effective mass is:

$$m_{eff} = \frac{m_i m_j}{\left(m_i + m_j\right)} = \frac{4\pi R_i^3 \rho \beta^3}{3\left(1+\beta\right)} \tag{4}$$

The effective radius is

$$R_{eff} = \frac{R_i R_j}{\left(R_i + R_j\right)} = \frac{R_i \beta}{1+\beta} \tag{5}$$

Inserting Equations 4 and 5 in Equation 3, and using dimensionless variables $\delta_n^* = \delta_n / R$, $\dot{\delta}_n^* = \dot{\delta}_n / v_0$, and $t^* = t / (R_i / v_0)$ yields:

$$K_1 \ddot{\delta}_n^* = \frac{(k_n \delta_n^*)}{(R_i \rho_P v_0^2)} + \frac{(c_n \dot{\delta}_n^*)}{(R_i^2 \rho_i v_0)}, \tag{6}$$

with $K_1 = 4\pi\beta^3 / \left[3\left(1+\beta^3\right)\right]$. Thus, scaling is based on dimensionless (normal) overlap for the translational motion of a particle, with the reference length being the parcel diameter in the parcel approach and the particle diameter in the original unscaled problem, i.e., the relative overlap will remain invariant when scaling the system. From Equation 4 the following dimensionless parameters can be identified:

$$\pi_1 = \beta,\ \ \pi_2 = \frac{k_n}{\left(R_i \rho_P v_0^2\right)},\ \ \pi_3 = \frac{c_n}{\left(R_i^2 \rho_P v_0\right)} \tag{7}$$

Condition π_1 requires a constant ratio of the radii of the colliding particles or parcels. This ratio will remain constant as long as each parcel is made up by the same number of particles N. π_2 requires that k_n/R_i = constant, since we require also the density and the reference velocity v_0 to be invariant. Condition π_3 requires c_n/R_i^2 to be constant [7].

1.3. Simple Shear Test

We started performing simple shear flow simulations in a cubic box (see Fig. 1). Lees-Edwards boundary conditions were used on two sides of the box. In the other sides periodic boundary conditions were employed. Initially linear spring model was used to reproduce the same data obtained by [7].

Shear rate was chosen such that $\gamma^* = \gamma d_{prim} / \sqrt{k / (\rho_P d_{prim})} = 10^{-4}$ was constant. Systems with different parcel sizes were investigated by holding the box size (0.015 m) and the primary particle diameter (100 um) constant, and grouping between 4 and 8192 particles in one parcel. For the inertial regime a solid fraction of $\Phi_P = 0.55$ was used. For the quasi-static regime a solid fraction of $\Phi_P = 0.62$ and 4000 parcels were used [3,7]. Simulations were performed using a 1) unscaled system and 2) scaled system according to previous obtained relation for stiffness and damping and data is shown in Fig. 2. For all simulations static friction used was 0.1, rolling friction 0.0, coefficient of restitution 0.75 and density 2500 kg/m^3.

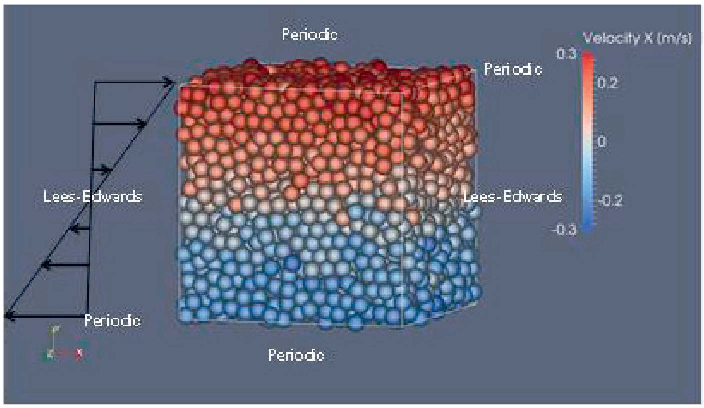

Fig. 1 – Shear box with boundary conditions indicated.

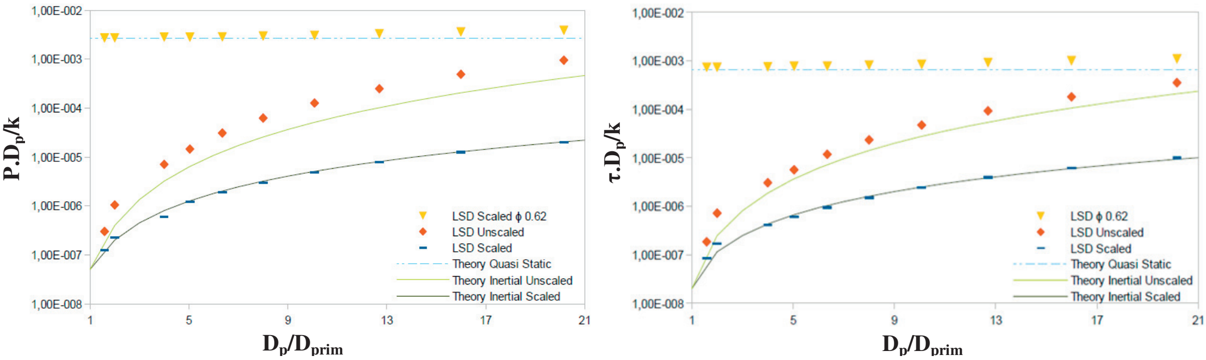

Fig. 2 – Pressure (left) and shear stress (right) for different parcels diameters. Data is displayed for scaled and unscaled system and predictive theory for each regime (quasi static and inertial) is also depicted.

We define pressure as $P = (\sigma_{xx}\sigma_{yy}\sigma_{zz})/3V$. Shear stress ($\boldsymbol{\tau}$) is defined as the stress component pointing in the shearing direction and acting on the surface normal to the gradient direction (the other components are much smaller).

2. Hertz Contact Model

We now extend the analysis from [7] by verifying the behavior of the Hertz contact model. [2] already performed some analysis in the behavior of Hertz model for quasi-static regime. We will also extend to the inertial regime. The difference between LSD and Hertz models is how stiffness and damping coefficients are calculated. In Hertz model stiffness is calculated as [5]:

$$k_n = \frac{4}{3} Y^* \sqrt{R^* \delta_n} \tag{8}$$

From Equation 8 we can observe that stiffness already scales with R. In his model the condition π_2 is satisfied. Damping coefficient is calculated as follow [5]:

$$\gamma_n = -2\sqrt{\frac{5}{6}}\beta\sqrt{S_n m^*} \tag{9}$$

and S_n is calculated as [5]:

$$S_n = 2Y^*\sqrt{R^*\delta_n} \tag{10}$$

We have then S_n which scales with R and multiplied by m* which scales with R^3. From Equation 10 we can see that damping scales with R^2 and satisfies condition π_3. From that we can observe that Hertz law is scale independent.

In the Hertz model stiffness is dependent of the overlap so it is not possible to define a fixed value as in the LSD model. However in the inertial regime the pressure is independent of the particle stiffness [3]. It is expected that pressure data obtained with Hertz contact model collapse in the same curve as the pressure data obtained by scaled LSD contact model. Also in the quasi-static regime it is expected that pressure increases with the increase of the stiffness. Although curves may not collapse (unless both models have equivalent stiffness) is expected a similar profile in the Hertz and scaled LSD curves. In fact this is depicted in Fig. 3. We considered for the simulations with Hertz contact model the same shear rate and volume fraction used for LSD model.

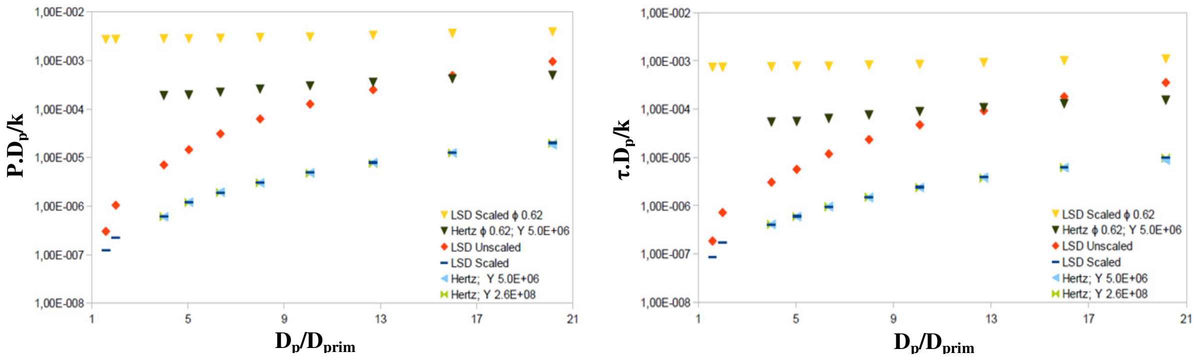

Fig. 3 – Pressure (left) and shear stress (right) for different parcels diameters. Hertz contact model data for different values of Young's modulus and LSD scaled are collapsed in the same curve in the inertial regime (bottom curve).

To verify the independency of the stiffness in the inertial regime and consistency in the profile of obtained data in the quasi static regime we varied the stiffness of the scaled LSD and also varied the Young's modulus in the Hertz contact model. Obtained data is depicted in Fig. 4.

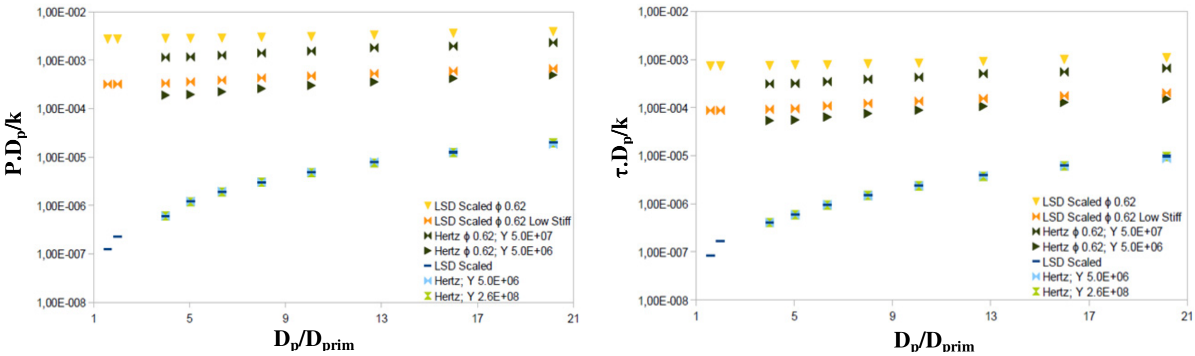

Fig. 4 – Pressure (left) and shear stress (right) for different parcels diameters. Hertz contact model for different Young's modulus values and LSD scaled for different values of stiffness quasi-static regime are depicted.

3. Cohesive contact model

With a defined method to evaluate the scalability of the contact models we proposed to extend the analysis for cohesive contact models. A limited number of tests were performed using a JKR contact model implemented in LIGGGGHTS software [5]. In JKR model normal force is calculated as [8]:

$$F_n = \frac{4E^* a^3}{3R^*} - \left(8\pi\xi E^* a^3\right)^{1/2} \tag{11}$$

where ξ is the surface energy and a is the particles contact area. Particle overlap is calculated as follows:

$$\delta_n = \frac{a^2}{R^*} - \left(\frac{2\pi\xi a}{E^*}\right)^{1/2} \tag{12}$$

When surface energy is zero, the second term of Equations 11 and 12 vanish and the JKR contact model reduces to standard Hertz contact model. The shear test failed for cohesive material and no predictive behavior could be obtained. We found that for high cohesive forces particles stick together and change the translational velocity. Also this additional cohesive force in the contact model may increase solid fraction in certain regions (depending on the particle stiffness) resulting in a different flow regime than initially modelled. On the other hand if cohesive forces are too low imposed velocity causes shear force to separate particles and the behavior is identical as Hertz contact law.

4. Conclusions

Coarse graining still needs more analysis to perform correct behavior in all particle flow regimes, even though this approach has been used for almost 20 years [1]. We performed a simple analysis in the linear spring dashpot model to obtain correlations in order to have a scale independent contact model. The same analysis was further extended to a Hertz contact model and a similar behavior was obtained for the Hertz and the scaled LSD contact model.

Although similar stresses were obtained for both contact models in different regimes both demonstrate a different behavior than the expected in terms of stresses when coarse graining modelling is to be used. For quasi-static regime was demonstrated that the stresses were almost constant for all parcel sizes. A slight increase is observed for correlations of D_p/D_{prim} >10 when dimensionless shear rate are > 10^{-2} [3]. This could be explained by the higher dimensionless shear rate for such parcels that results in flow regime where both inertial and quasi static flow merge in one curve and pressure increases linearly as shown by [3].

The inertial regime has a very different profile in the obtained pressure for different parcels size. The pressure increases significantly with the parcel size. In coarse graining we desire a constant pressure for different parcels size similar to the one obtained in the quasi static regime.

For coarse graining and especially in the inertial regime is necessary to develop correlations that corrects this increase in pressure. A relaxation function was implemented by [7] for LSD models to try minimize this increase in pressure. As further steps a relaxation function will be implemented in Hertz contact model to try to obtain a generalized function that could be valid for the different regimes.

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