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Determination of the normal spring stiffness coefficient in the linear spring–dashpot contact model of discrete element method

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ABSTRACT

The discrete element method is a method for simulation of a particle system. For the "soft-sphere" mechanism of particle interactions, there are several models for normal contact forces, namely linear spring–dashpot, and non-linear damped Hertzian spring–dashpot, among others. The focus of this paper is to determine the normal spring stiffness coefficient of the linear model through the numerical solution for the overlap between particles in non-linear models. The linear spring stiffness is determined using equivalence between the linear and the nonlinear models. Using the MFIX computational code, the proposed approach is applied in the numerical simulations of two problems: single freely falling particle and bubbling fluidized bed. A method based on mean dimensionless overlap is suggested as an initial estimate to determine the normal spring stiffness coefficient. Other possible methods for computing the stiffness coefficient are also discussed in this work, e.g., maximum dimensionless overlap and dimensionless contact duration.

1. Introduction

The modeling of particulate systems has been an important focus of research worldwide, as these are fairly common in nature, such as rain drops in air, snowfall, and several industrial processes. Examples of the latter include: riser reactors; bubble column reactors; liquidized bed reactors; scrubbers; and dryers, among others. Applications of modeling of granular flows are usual in dune erosion, in processing pharmaceutical powders, and in industrial mills, among others. The behavior of those flows can be predicted experimentally, theoretically, and computationally. In some cases, the laboratory model needs to have a scale that is different from an original plant. In such case the theoretical or computational model can be a tool for extrapolation to the scale of the problem.

In gas–solid flow problems, the continuum equations can be solved for both phases and it is called Eulerian–Eulerian or two-fluid method. When the gas phase is considered as a continuum and the dispersed phase as discrete, the approach is called Eulerian–Lagrangian.

Alder and Wainwright [1] introduce the molecular dynamic methods as a methodology to study the macroscopic behavior of particles. The techniques developed for molecular dynamics can be adapted to discrete particle models, including the formulation of particle–particle interactions. The molecular dynamics model together with the contact mechanisms is a method called discrete element method (DEM). The discrete element method approach has been applied in several areas, e.g., in geotechnical mechanics by Cundall and Strack [2], pneumatic transport technology by Tsuji et al. [3], fluidized beds by Tsuji et al. [4], tumbling ball mills by Mishra and Rajamani [5], segregation of granular materials by Ketterhagen et al. [6], cohesive particles flows by Weber [7], and solids mixing in gas-fluidized beds by Rhodes et al. [8], among other studies. A comprehensive literature review is found in the works published by Zhu et al. [9,10], which summarize the studies based on discrete particle simulation.

The assumption in DEM is that during a small time step, the disturbances cannot propagate from any particle to others except to its immediate neighbors. Based on the mechanism of particle interaction, the contact forces can be modeled either as "hard-sphere" or as "soft-sphere" [11]. The contact forces are included in the Newton's second law of motion to determine the dynamic of the particles. In a hard-sphere model, the trajectories of particles are determined by momentum conserving binary collisions. Campbell and Brennen [12] reported the first hard-sphere discrete particle simulation used to study granular systems. Several studies have been developed using the hard-sphere model. A discrete particle simulation using a hard-sphere model of a bubble and slug formation in a two-dimensional gas-fluidized bed has been developed by Hoomans et al. [13]. Goldschmidt et al. [14] made a comparison between hard-sphere model, two-fluid model and experiments in a pseudo-two-dimensional gas-fluidized bed. Lu et al. [15] investigated solid motions in a two-dimensional bubbling fluidized bed using discrete hard-sphere model. Müller and Pöschel [16] pointed out some limitations of hard-sphere model for granular dynamics depending on the material and system parameters.

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In soft-sphere models, the particles are allowed to overlap slightly and the contact forces are subsequently calculated from the deformation history of the contact using a contact-force scheme. The soft-sphere method for granular dynamics simulations was developed by Cundall and Strack [2]. In the soft-sphere approach there is a mapping between the contact forces during the impact and dynamic systems. A detailed study for the impact theory is found in the book by Goldsmith's [17]. The elastic mechanism in the impact modeling is first given by Hertz [18,19]. Timoshenko and Goodier [20] give a classical presentation of theory of elasticity. The energy lost during impact can be associated with damping mechanisms during the contact period. Simo and Hughes [21] present the theoretical foundations of inelasticity, its numerical formulation, and a description of computational algorithms for classical plasticity, viscoplasticity, and viscoelasticity material models. Several schemes have been proposed in the literature for modeling the contact-force, such as the one proposed by Walton and Braun [22] that uses two different spring constants to model the energy dissipation in the normal and tangential directions to examine the effects of inelasticity and friction on shearing two-dimensional assemblies of disks. Hunt and Crossley [23] discuss the Kelvin–Voigt model and introduce a new non-linear damping term for the impacts between solid bodies. Yigit et al. [24] compare spring–dashpot models for impact modeling with experimental data for a radially rotating flexible beam.

The linear model for contact forces is widely used in DEM simulations (see e.g. [25–29]). The main reason is that the model is simple with analytic solution for the collision parameters, and this model is less computationally expensive comparing to the non-linear models. In the linear method, we need to specify values for the spring stiffness and damping coefficients. Shäfer et al. [30] describe that in principle, the linear spring dashpot model has no free parameters, since spring stiffness and damping coefficients can be set adjusting normal restitution coefficient and contact duration to the corresponding experimental values exhibited by a given material in a velocity range. The relationships for spring stiffness and damping coefficient can be derived as a function of the normal restitution coefficient and contact duration (e.g. Hoef et al. [26], Shäfer et al. [30]). Stevens and Hrenya [31] discussed criteria to choose typical input parameters (e.g., spring constant and dashpot coefficient) based on an equivalent estimated collision time. This approach is preferred for dense systems which lead to large contact times ([31,32]).

For the linear model, in case we only have the value of normal restitution coefficient, we can compute only the damping coefficient for the linear method using an analytic expression (see Shäfer et al. [30]). The value for the stiffness coefficient can be estimated by using known numerical experiments, or other approach, such as equivalence between linear and non-linear models. In the literature, there are various non-linear models for prediction of collision parameters during normal impacts (e.g. Tsuji et al. [3], Hunt and Crossley [23], Kuwabara and Kono [33]). The conservative elastic force in these models is computed based on Hertz's theory ([18,19]) and the non-linear stiffness coefficient can be estimated with material properties as Young modulus and Poisson ratio. The basic difference between these non-linear models is the computation of the non-conservative damping force. Tsuji et al. [3] consider a damping force proportional to the fourth-root of the overlap for simulating cohesionless particles in a horizontal pipe. Hunt and Crossley [23] consider a continuous force at the start and the end of the contact. Kuwabara and Kono [33] proposed a damping force proportional to the square-root of the overlap for the collision of viscoelastic spheres.

There are several studies that present equivalence between linear and non-linear models. Lan and Rosato [34] use an equivalent maximum strain energy for a linear normal loading stiffness evaluation. The authors assume that the incident kinetic energy is stored in Hertzian elastic strain energy and the normal loading stiffness is obtained when this nonlinear strain energy is equated to the linear strain energy. Lan and Rosato [35] use a limited overlap approach for determining the stiffness coefficient. The linear normal loading stiffness value is associated with the maximum normal overlaps between contacting spheres, for example, an overlap based on percentage of the particle diameter. Dury and Ristow [36] also determine a value for linear normal stiffness based on a limited overlap computed by a percentage of the sum of radii of two particles. Buchholtz and Pöschel [37] relate the linear normal stiffness with Young modulus characterizing the elastic restoration of the spheres. Antypov and Elliott [38] map the non-linear spring–dashpot model onto the linear model adjusting the linear spring constant with nonlinear ones.

The focus of this paper is to determine the normal spring stiffness coefficient of the linear model through the numerical solution for the overlap between particles in non-linear models. The linear spring stiffness is determined using equivalence between the linear and the nonlinear models. The equivalence process can be performed by three methods, i.e., maximum dimensionless overlap, dimensionless contact duration, and mean dimensionless overlap. Using the MFIX code, the proposed approach is applied in the numerical simulations of two problems: (a) single freely falling particle; and (b) bubbling fluidized bed. In the problems analyzed in this work (simple contact between particle–particle and particle–wall and monodisperse gas–solid flows), a method based on mean dimensionless overlap is suggested as an initial estimate to determine the normal spring stiffness coefficient.

2. Gas–solid mathematical model

The open source code MFIX ("Multiphase Flow with Interphase eXchanges") [39,40] developed at NETL ("National Energy Technology Laboratory") has been widely used to simulate hydrodynamics, heat transfer and chemical reactions occurring in bubbling and circulating fluidized beds. The gas-phase can be treated as continuum and modeled by the fundamental equations of mass and momentum conservation. The solid phases can be modeled as a continuum phase in a two-fluid model (TFM) where constitutive relations for the transport coefficients are given in terms of hydrodynamic variables. Enwald et al. [41] and Ishii and Hibiki [42] present a description to derive a closed two-fluid model applicable to non-reacting gas–solid flows. The solid stress equation in viscous regime can be modeled based on Kinetic Theory for Granular Flows (KTGF) (see Lun et al. [43], Gidaspow [44], Agrawal et al. [45]). In the plastic flow regime, the solid stress can be described by adopting theories from the study of soil mechanics (see [46–49]). Recently, a constitutive model with microstructure evolution for flow of rate-independent granular materials has been developed by Sun and Sundaresan [50]. An overview of the granular material flows is found in the work of Campbell [51]. The solid phases can also be treated as disperse phases (see Tsuji et al. [3]). In this case, the solid phases are represented by particles and the motion of the particles is modeled by the solution of Newton's law applied in each particle. MFIX code is used in this work for the numerical simulations and this code supports both approaches: Two-fluid method (TFM) ([39,40]) and fluid-DEM approach ([27,52,53]). Next, we describe the governing equations for the latter approach (Eulerian–Lagragian or fluid-DEM) used in the present work.

Considering an isothermal gas–solid flow without chemical reactions, the mass, momentum, and constitutive equations for the gas phase are formulated as follows. The continuity equation for the gas phase is:

$$\frac{\partial}{\partial t}\left(\epsilon_g \rho_g\right) + \nabla \cdot \left(\epsilon_g \rho_g \mathbf{v}_g\right) = 0 \qquad (1)$$

where ϵ_g, ρ_g and $\mathbf{v}_g$ are respectively the gas-phase void fraction, the density of gas phase and the gas-phase velocity.