Influence of soft and rigid contact models on granular dynamics

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We compare in the weak form, the efficiency and accuracy of the compliant and rigid contact models. The first approach, also known as "discrete element method via penalty" or simply DEM-P, is commonly used in the soft matter physics and geomechanics communities; it can be traced back to the work of Cundall and Strack [1, 2]. The second approach, called DEM-C from "complementarity", considers the grains perfectly rigid and enforces non-penetration via complementarity conditions; it is commonly used in robotics and computer graphics applications and had two strong promoters in Moreau and Jean [3, 4]. DEM-P and DEM-C are manifestly unlike each other – they use different (*i*) approaches to model the frictional contact problem; (*ii*) sets of model parameters to capture the physics of interest; and (*iii*) classes of numerical methods to solve the differential equations that govern the dynamics of granular materials. Our study of granular materials was composed of five experiments: shock wave propagation, cone penetration, direct shear, triaxial loading, and hopper flow, which we used to compare the DEM-P and DEM-C solutions.

DEM-P and DEM-C: method summary. DEM-P is a regularization method introduced to replace a finite element analysis at each contact point [1, 2, 5, 6]. It relies on a relaxation of the rigid-body assumption and a *surrogate deformation* of two bodies in mutual contact Although the shapes might be overly complex, it is customary to combine the surrogate deformation with the Hertzian theory, which is only applicable for a handful of simple scenarios such as sphere-to-sphere or sphere-to-plane contact, see for instance [5], in order to yield a general methodology for computing the normal (F_n) and tangential (F_t) forces at the contact point. As an example, a viscoelastic model based on Hertzian contact theory, which was used for the current study, takes the form

$$F_n = \sqrt{\bar{R}\delta_n}\,(K_n\delta_n - C_n\bar{m}\mathbf{v}_n) \tag{1a}$$
$$F_t = \sqrt{\bar{R}\delta_n}\,(-K_t\boldsymbol{\delta}_t - C_t\bar{m}\mathbf{v}_t)\ , \tag{1b}$$

in normal, n, and tangential, t, directions, respectively. Herein, $\boldsymbol{\delta}$ is the overlap of two interacting bodies; $\bar{R}$ and $\bar{m}$ represent the effective radius of curvature and mass, respectively; and $\mathbf{v}$ is the relative velocity at the contact point. For the materials in contact, the normal and tangential stiffness and damping coefficients K_n, K_t, C_n, and C_t are obtained, through various constitutive laws, from physically-measurable quantities, such as Young's modulus, Poisson ratio, and the coefficient of restitution [5].

DEM-C takes a different tack; it draws on a complementarity condition that imposes a non-penetration unilateral constraint, see Eq. (2a). That is, for a potential contact i in the active contact set $\mathscr{A}(\mathbf{q}(t))$, either the gap Φ_i between two geometries is zero and consequently the normal contact force $\widehat{\gamma}_{i,n}$ is greater than zero, or vice-versa. The Coulomb friction model is posed via a maximum dissipation principle [7], which for contact i involves the friction force components $(\bar{\gamma}_{i,w}, \bar{\gamma}_{i,u})$ and the relative motion of the two bodies in contact, see Eq. (2b). The frictional contact force associated with contact i leads to a set of generalized forces, shown with an under-bracket in Eq. (2c), which are obtained using the projectors $\mathbf{D}_{i,n}$, $\mathbf{D}_{i,u}$, and $\mathbf{D}_{i,w}$, see, for instance, [8]. This leads in Eq. (2) to a so called differential variational inequality problem [7]

$$0 \leq \Phi_i(\mathbf{q}) \perp \widehat{\gamma}_{i,n} \geq 0 \tag{2a}$$

$$(\widehat{\gamma}_{i,u}, \widehat{\gamma}_{i,w}) = \underset{\sqrt{\bar{\gamma}_{i,u}^2 + \bar{\gamma}_{i,w}^2} \leq \mu_i \widehat{\gamma}_{i,n}}{\operatorname{argmin}} \quad \mathbf{v}^T \left(\bar{\gamma}_{i,u} \mathbf{D}_{i,u} + \bar{\gamma}_{i,w} \mathbf{D}_{i,w} \right) \tag{2b}$$

$$\mathbf{M}(\mathbf{q})\dot{\mathbf{v}} = \mathbf{f}(t, \mathbf{q}, \mathbf{v}) + \mathbf{G}(\mathbf{q}, t)\hat{\lambda} + \sum_{i \in \mathscr{A}(\mathbf{q})} \underbrace{\left(\widehat{\gamma}_{i,n} \mathbf{D}_{i,n} + \widehat{\gamma}_{i,u} \mathbf{D}_{i,u} + \widehat{\gamma}_{i,w} \mathbf{D}_{i,w} \right)}_{i^{th} \text{ frictional contact force}} . \tag{2c}$$

Numerical experiments. For the purpose of quantifying the similarities and differences of DEM-P and DEM-C we used open-source software package, Chrono [9, 10], that implements both approaches. We considered five benchmark tests, including a wave propagation experiment, a cone penetration test, a direct shear test, a triaxial test and a hopper flow analysis. The metrics of interest in this DEM-P vs. DEM-C comparison were solution accuracy, robustness, and required computational effort as reflected in simulation run times.

Conclusion. This exercise helped us reach two conclusions. First, both DEM-P and DEM-C are predictive; i.e., they predict well the macro-scale emergent behavior by capturing the dynamics at the micro-scale. Second, there are classes of problems for which one of the methods has an upper hand. Unlike DEM-P, DEM-C cannot capture shock-wave propagation through granular media. However, DEM-C is proficient at handling arbitrary grain geometries and solves at large integration step sizes smaller problems; i.e., containing thousands of elements, very effectively. The DEM-P vs. DEM-C comparison was carried out using a public-domain, open-source software package; the models used are available on-line.

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