USING LIGGGHTS FOR PERFORMING DEM SIMULATIONS OF PARTICLES OF COMPLEX SHAPES WITH THE MULTISPHERE METHOD

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The multisphere method is commonly used as an approximation for modeling particles of complex geometric shapes in DEM simulations. However, typically the mass and moment of inertia of the resulting sphere clumps are incorrectly computed as a result of the (artifactual) contribution of the sphere-sphere overlaps. We adapted the current public release of LIGGGHTS in order to perform DEM simulations of rigid bodies using the mass and moment of inertia of the particles as obtained through an analytical (exact) method.

INTRODUCTION

Many particulate systems occurring in nature or in industrial applications are made of particles which have complex geometric shapes. The correct modeling of particle shape in DEM simulations is important for accurately predicting the interaction between the particles as well as the dynamic behavior of the system.

The multisphere method, which consists of combining spheres of different sizes to build a rigid body (sphere clump), is a widely used method for approximating complex particle shapes in DEM simulations [1-5]. However, this method suffers from an obvious deficiency that is not considered in most numerical simulations: both the mass and moment of inertia of the clumps incorporate the excess (artifactual) contribution from the sphere-sphere overlaps. Indeed, one can calculate the mass and moment of inertia of each clump numerically, e.g. using Monte Carlo [5]. Evidently, such a calculation can become computationally too expensive if the system contains a large number of particles. Some authors proposed to adjust the density of the spheres constituting the clumps in such a manner to obtain the target mass and moment of inertia [4]. However, using the correct density of the particle's material is essential in order to correctly model inter-particle collisional forces.

Here we compute the mass and moment of inertia of each complex particle analytically, by explicitly removing the excess contribution due to the overlaps between constituent spheres within the clump. We have adapted the current public release of LIGGGHTS [7] in order to allow us to perform the numerical simulations using the exact results of these analytical calculations. In the next section we present the equations we use to compute the mass and moment of inertia of the sphere clumps. These equations are applicable when sphere-sphere overlaps within a rigid body involve not more than two spheres. We then discuss an example of numerical simulations that illustrates the relevance of the correction in the particles' mass and moment of inertia for the dynamic behavior of a granular system made of particles of complex geometric shape.

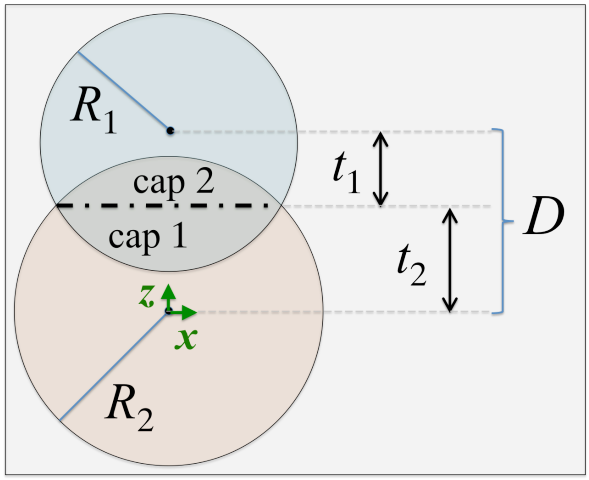

Fig 1. Schematic diagram of a sphere-sphere overlap within a clump (rigid body). D is the distance between the centers of the overlapping spheres, which have radii R_1 and R_2. t_1 and t_2 denote the respective distances from each sphere's center to its cap base.

ANALYTICAL EQUATIONS

We consider two overlapping spheres within a rigid body, the centers of which are separated by a distance D (Fig. 1). The overlapping spheres are labeled 1 and 2. The contribution of the sphere-sphere overlap to the mass and moment of inertia of the rigid body is computed for all pairs of constituent spheres in the clump for which $D < R_1 + R_2$. The mass m_{overlap} of the sphere-sphere overlap is the sum of the masses of caps 1 and 2 ($m_{\text{cap 1}}$ and $m_{\text{cap 2}}$, respectively), whereas the mass of each cap is given by the equation,

$$m_{\text{cap }k} = \left[\rho_{\text{p}}\pi/3\right]\cdot\left[3R_k\ell_k^2 - \ell_k^3\right], \tag{1}$$

with ρ_{p} standing for the material's density and $k = 1, 2$, whereas $\ell_k = R_k - t_k$ Moreover, we calculate the moment of inertia of the caps by considering, firstly, the case where the vector $\mathbf{D} = \mathbf{r}_1 - \mathbf{r}_2$ (where $\mathbf{r}_k$ is the center-of-mass position of sphere k) is parallel to the z axis (Fig. 1). In this case, the moment of inertia tensor of each cap k ($\hat{\text{I}}_{\text{cap }k}$) is diagonal with components given by (see also Ref. [6], which uses these equations for DEM simulations of pharmaceutical tablets),

$$\begin{aligned} I_{xx,\text{ cap }k} = I_{yy,\text{ cap }k} &= \left[\rho_{\text{p}}\pi/4\right]\cdot\left[4R_k^3\ell_k^2 - \frac{16R_k^2\ell_k^3}{3} + 3R_k\ell_k^4 - \frac{3}{5}\ell_k^5\right] + \\ &+ m_{\text{cap }k}\left[\left(L_{\text{overlap }k} - L_{\text{ctrd }k}\right)^2 - L_{\text{ctrd }k}^2\right], \end{aligned} \tag{2}$$

$$I_{zz,\text{cap}k} = \left[\rho_{\text{p}}\pi/2\right]\cdot\left[\frac{4}{3}R_k^2\ell_k^3 - R_k\ell_k^4 + \frac{1}{5}\ell_k^5\right]. \tag{3}$$

In Eq. (2), $L_{\text{centr }k}$ is the geometric centroid of cap k; it is computed relative to the center of sphere k. Furthermore, $L_{\text{overlap }k}$ is the distance between the center of sphere k and the center of mass of

the total overlap volume which comprises caps 1 and 2. The tensor of inertia $\hat{\mathrm{I}}_{\mathrm{overlap},z}$ of the sphere-sphere intersection is then given by $\hat{\mathrm{I}}_{\mathrm{overlap},z} = \hat{\mathrm{I}}_{\mathrm{cap\ 1}} + \hat{\mathrm{I}}_{\mathrm{cap\ 2}}$. We note that this equation considers that **D** is parallel to the *z* axis (Fig. 1). The tensor of inertia $\hat{\mathrm{I}}_{\mathrm{overlap}}$ for the case in which **D** makes an angle φ with the *z* axis reads, $\hat{\mathrm{I}}_{\mathrm{overlap}} = \hat{R}\hat{\mathrm{I}}_{\mathrm{overlap},z}\hat{R}^{-1}$, where $\hat{R}$ is the rotation matrix associated with the rotation of a vector by an angle φ around the axis $\mathbf{e}_{\mathrm{D}} \times \mathbf{e}_z$, with $\mathbf{e}_{\mathrm{D}} = \mathbf{D}/|\mathbf{D}|$.

We then calculate the body's total mass m_{body}, center-of-mass position $\mathbf{r}_{\mathrm{cm}}$ and inertia tensor $\hat{\mathrm{I}}_{\mathrm{body}}$ using the values of the mass (m_{overlap}) and tensor of inertia ($\hat{\mathrm{I}}_{\mathrm{overlap}}$) obtained as described above. The equations for m_{body} and $\mathbf{r}_{\mathrm{cm}}$ write,

$$m_{\mathrm{body}} = \sum_{i=1}^{N_s} m_{\mathrm{sphere}\,i} - \sum_{j=1}^{N_o} m_{\mathrm{overlap}\,j}, \tag{4}$$

$$\mathbf{r}_{\mathrm{cm}} = m_{\mathrm{body}}^{-1}\left[\sum_{i=1}^{N_s} m_{\mathrm{sphere}\,i}\mathbf{r}_i - \sum_{j=1}^{N_o} m_{\mathrm{overlap}\,j}\mathbf{r}_j\right], \tag{5}$$

where N_{s} and N_{o} denote, respectively, the number of spheres and caps pairs in the body, while $\mathbf{r}_{i(j)}$ denotes the center-of-mass position of sphere *i* (caps pair *j*). Moreover, $\hat{\mathrm{I}}_{\mathrm{body}}$ reads,

$$\hat{\mathrm{I}}_{\mathrm{body}} = \sum_{i=1}^{N_s} \frac{2}{5} m_{\mathrm{sphere}\,i} R_i^2 \hat{1} - \sum_{j=1}^{N_o} \hat{\mathrm{I}}_{\mathrm{overlap}\,j} + \hat{\mathrm{A}}, \tag{6}$$

where $\hat{\mathrm{A}}$ is the inertia tensor associated with the discrete distribution of mass elements m_k, each representing either a caps pair or a sphere. That is,

$$\hat{\mathrm{A}} = \sum a_k m_k \begin{bmatrix} Y_k^2 + Z_k^2 & -X_k Y_k & -X_k Z_k \\ -X_k Y_k & X_k^2 + Z_k^2 & -Y_k Z_k \\ -X_k Z_k & -Y_k Z_k & X_k^2 + Y_k^2 \end{bmatrix}, \tag{7}$$

where $a_k = 1$ (−1) for spheres (caps pairs), while X_k, Y_k, Z_k are the distances between the center-of-mass of element *k* and the body's principal axes. The inertia tensor is then diagonalized by performing a principal axis transformation. The normalized eigenvectors obtained from this transformation yield the orthogonal transformation matrix $\hat{\mathrm{J}}$. Using this matrix, a vector **u** in the body's fixed frame of reference is transformed to the inertial frame through the equation, $\mathbf{u}_{in} = \hat{\mathrm{J}}\mathbf{u}$.

Finally, the motion of the rigid body is computed by numerically solving the equation,

$$m_{\mathrm{body}}\ddot{\mathbf{r}}_{\mathrm{cm}} = \sum_{i=1}^{N_s} \mathbf{F}_i + m_{body}\mathbf{g}, \tag{8}$$

where **g** is gravity and $\mathbf{F}_i$ is the total force on the *i*-th constituent sphere of the clump, where the forces considered in the calculation of $\mathbf{F}_i$ are due to collisions with particles belonging to other rigid bodies. Furthermore, the resultant torque **M** on the rigid body is given by,

$$\mathbf{M} = \sum_{i=1}^{N_s} \left(\mathbf{r}_i - \mathbf{r}_{\mathrm{cm}}\right) \times \mathbf{F}_{t,i}, \tag{9}$$

where $\mathbf{F}_{t,i}$ is the tangential force on the body's i–th constituent sphere, while the angular velocity of the body, $\vec{\omega}$, evolves according to the Euler's equations in the body's fixed frame, $\hat{I}\dot{\vec{\omega}} + \vec{\omega} \times (\hat{I}\vec{\omega}) = \hat{J}^{-1}\mathbf{M}$.

DISCUSSION

It is clear that simulations using the multisphere method should account for the correct computation of the particles' mass and moment inertia. However, it is interesting to discuss an example of numerical simulations where the effect of the error due the usual approximation (of neglecting the artifactual contributions due to sphere-sphere overlaps) on the macroscopic dynamic behavior of the system is visible.

We consider a granular gas of 864 perfectly elastic particles, each made of two spheres of equal size, evolving within a cubic box with periodic boundary conditions. The density of the spheres constituting each rigid body is $\rho_p = 1140$ kg/m^3, their Young modulus is $Y = 10^7$ Pa and their Poisson ratio $\nu = 0.40$. Both constituent spheres of the clump have diameter $d_s = 13.33$ cm and are separated by a distance $D = d_s/2$. The volume fraction of the granular system is 0.001 and the total kinetic energy is about 3.24 kJ.

We also perform a simulation using spheres of diameter $d_L = 20$ cm. Each sphere has the same material properties as the rigid bodies but its mass is set equal to m_{body}, i.e. the mass of the rigid body computed analytically (with Eq.(4)).

The simulations are performed using the Hertz-Mindlin model to compute the normal collisional forces between the particles [7]. We assume no damping and no tangential forces. Thus, the spherical particles do not display rotational motion, while the rigid bodies do. In Fig. 2 we compare the values of mean-square displacement (msd) calculated for the system of spherical particles (dotted line) with the ones obtained for the two-sphere clumps with the correct (continuous line) and wrong (dashed line) values of mass and moment of inertia.

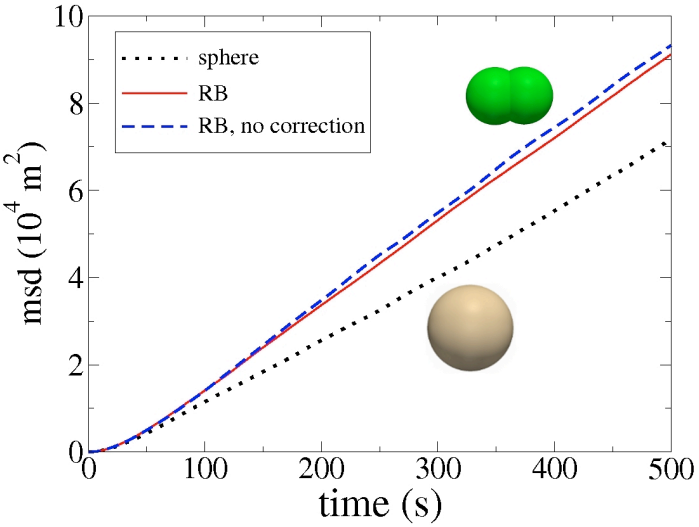

Fig 2. The continuous line shows the mean-square displacement (msd) obtained using the analytical equations to compute the correct values of the mass (m_{body}) and moment of inertia of the complex particles (rigid bodies modeled here as two-sphere clumps). The dashed line denotes the result obtained with the multisphere method without performing the correction. The dotted line gives the msd for a sphere which has the mass m_{body}.

As we can see in Fig. 2, the values of mean-square displacement of the rigid bodies calculated without the correction differ from the ones obtained with the correct calculation of the particles' mass and moment of inertia. Although the difference is small (about 10% of the difference between the respective msd's of spherical particles and rigid bodies), certainly the error should depend on the particle shape. While we have chosen the simplest configuration of two-sphere clumps in this preliminary study, in the future these simulations should be extended in order to account for more complex geometric shapes using a larger number of particles to build the clumps. Also it could be helpful to analyze the separate effects of correcting the mass or the moment of inertia on the results.

CONCLUSION

We presented analytical equations for computing the mass and moment of inertia of particles of complex geometric shapes built with the multisphere method, which can be used when sphere-sphere overlaps within each clump involve not more than two spheres. The mass and moment of inertia of each complex particle are computed by explicitly removing the excess (artifactual) contribution of the sphere-sphere intersections. We adapted the current public release of LIGGGHTS [7] in order to allow us to perform molecular-dynamics simulations using the results obtained from these analytical calculations. We discussed an example of a granular system where the effect of the error arising from the usual approximation (of not excluding the artifactual contributions of the sphere-sphere overlaps) on the dynamic behavior of the system is visible.

ACKNOWLEDGMENTS

We thank Thorsten Pöschel, Patric Müller, Dan Serero, Severin Strobl and Aldo Glielmo for discussions and helpful suggestions. We also thank Patric Müller for kindly sending a set of initial particle positions and translational velocities for the granular gas simulations. We acknowledge support from the German Research Foundation (DFG) within the frame of the Collaborative Research Initiative "Additive Manufacturing" (SFB 814) and through the Cluster of Excellence "Engineering of Advanced Materials".

REFERENCES

1. J. A. C. Gallas and S. Sokolowski, *Int. J. Mod. Phys.* **7**, 2037-46 (1993).
2. T. Pöschel, T. Schwager, *Computational Granular Dynamics,* Springer, 2004.
3. X. Garcia, J. -P. Latham, J. Xiang, P. Harrison, 'A clustered overlapping sphere algorithm to represent real particles in discrete element modelling', *Geotéchnique* **59**, 779-784 (2009).
4. J. F. Ferellec, G. R. McDowell, 'A method to model realistic particle shape and inertia in DEM', *Granular Matter* **12**, 459-67 (2010).

5. S. Amberger, M. Friedl, C. Goniva, S. Pirker, C. Kloss, ‘Approximation of objects by spheres for multisphere simulations in DEM’, in *ECCOMAS-2012*, edited by J. Eberhardsteiner et al.
6. M. Kodam, J. Curtis, B. Hancock, C. Wassgren, ‘Discrete element method modeling of bi-convex pharmaceutical tablets: Contact detection algorithms and validation’, *Chemical Engineering Science* **69**, 587-601 (2012).
7. C. Kloss, C. Goniva, A. Hager, S. Amberger, S. Pirker, ‘Models, algorithms and validation for open-source DEM and CFD-DEM’ *Progr. Comput. Fluid Dy.* **12**, 140-52 (2012); http://www.liggghts.com.