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QUANTIFYING ERRORS DUE TO THE HERTZIAN CONTACT MODEL IN MULTI-SPHERE DISCRETE ELEMENT MODELLING SIMULATIONS

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Abstract. In Discrete Element Modelling (DEM), non-spherical particles are often emulated using clusters of rigidly connected spheres that can be either overlapping or not. Within this multi-spherical approach, two sources of error directly affecting the normal contact forces present can be identified. One is due to the difference between the true particle shape and the multi-spherical approximation; the other arises from the contact model used in the DEM simulations. The potential for inaccuracy in multi-sphere DEM simulations is well known. However, for a DEM simulator it remains unclear what error might be expected when multi-sphere particles are adopted. This contribution focuses on the role of the contact model as a source of error for the special case of two-sphere particles.

Considering a single multi-spherical rod consisting of two identical spheres and quasi-statically compressing it until a total of 5% strain has been applied, the force response obtained through Finite Element Analysis (FEA) was compared against the Hertzian contact model. The process was repeated for spheres with varying degrees of overlap, ranging from 0 to 100%, and the relative errors of the FEA models against the Hertzian contact model were calculated.

Up to a 60% sphere overlap, Hertz underpredicts the normal contact forces beyond 0.5% strain, where the disparity between the FEA model and Hertz forces is increasing monotonically with strain. However, beyond an overlap of 70%, Hertz overpredicts the normal contact forces with the sphere overlap being the main driver of this deviation. Future research will involve comparing these errors with the 'shape' source of error by compressing perfect spherocylinders, considering rods composed of more spheres, and investigating how the error is affected by the relative orientation of two contacting particles.

1 Introduction

The Discrete Element Method (DEM) has progressed significantly since it was first introduced by Cundall and Strack [1]. In the 'soft-particle' DEM approach, a contact model is needed to relate finite interparticle overlaps to the force. Regardless of particle shape, these contact models are usually based on Hooke's law, i.e., the normal component of contact force is proportional to the overlap, or Hertzian mechanics [2]. Although sophisticated contact models have been developed recently for non-spherical particle simulations [3, 4], the overwhelming majority of non-spherical simulations still use Hooke or Hertz.

One popular way of representing non-spherical granules in DEM simulations is using multi-spherical clusters. A cylindrical granule for instance can be emulated by fixing together a number of collinear spheres. The constituent spheres may be overlapping or even have different diameters, thus permitting virtually any shape to be reproduced.

Nevertheless, two sources of error can be identified by using this multi-spherical approach, that directly affect the normal contact forces present in particle collisions. The first one stems from the difference between the actual particle shape and its multi-spherical approximation. Although similar, the multi-spherical cluster will always be a mere approximation of the true particle. The second source of error arises from the contact model used in the DEM simulations since in such cases a contact model developed for spheres is usually adopted, even though the original granule that is emulated is not a sphere. There is a case to be made about an additional source of error coming from the Poisson effect, which may be considerable at Poisson's ratios approaching 0.5 [5]. In this study however, the error stemming from the Poisson's ratio effect was considered negligible compared to the other two sources of error identified, as a value of 0.3 was used. While the potential for inaccuracy when using the multi-spherical approach is well known [6, 7], to the authors' knowledge, there is no rigorous quantification of the errors present. This is what is being addressed in this piece of work.

The Finite Element Method (FEM) was used to quantify the errors present when using a contact model designed primarily for spheres, such as Hertz [2], in non-spherical particle DEM simulations. First, the simulation approach was verified by comparing with the analytical solutions of Hertz [2] and Tatara [8] for the uniaxial compression of an elastic sphere. Then the focus was shifted towards the uniaxial compression of two-sphere rods in order to examine how the sphere overlap affects the normal contact force when such multi-spherical rods collide in parallel to each other.

2 Method – Finite Element Analysis

2.1 Verification – Uniaxial compression of a sphere

The verification closely follows the process outlined in Constandinou and Hanley [5]. The commercial software Abaqus [9] was used to quasi-statically compress a sphere between two rigid plates as shown in Figure 1. The granule and material properties match the ones used by Rathbone et al. [10], albeit ignoring plasticity. Those include a radius R of 0.1 mm, Young's modulus E of 6.1 GPa and Poisson's ratio ν of 0.3.

In order to replicate the granule conditions from a DEM simulation, the granule was modelled as an elastic body using the inbuilt routine in Abaqus for isotropic materials which requires only the Young's modulus and Poisson's ratio. An octant of the entire sphere was simulated using three planes of symmetry and 2196 linear 'C3D8R' elements as shown in Figure 2. The mesh was refined at the point of contact to properly capture the normal force acting on the rigid plate. Following a mesh dependence study which also included meshing with quadratic elements, the selected mesh was deemed sufficient as the difference in the results was of the order of 0.1–0.2%. The use of linear elements was favoured in order to keep the comparison with further research involving dynamic collisions consistent.

The sphere deformation in the simulation was obtained from the plate displacement, while the normal contact force was obtained from the reaction force applied on the plate. The compression was stopped when the total deformation applied reached an axial strain of 5%: a common heuristic for the maximum permissible overlap between spheres in DEM simulations as well as the limit to Abaqus' inbuilt elastic material model routine [9]. The results were compared with the predictions of Hertz [2] and Tatara [8]. The comparison with the latter allows the reliability of these implicit simulations to be verified against an analytical solution developed for non-infinitesimal strains.

According to Hertz, the normal contact force, F, for a sphere in contact with a rigid plate is:

$$F = \frac{4E\sqrt{R}}{3\left(1-\nu^2\right)}\delta^{\frac{3}{2}} \tag{1}$$

where δ is the deformation of the sphere. The equivalent relationship between the normal contact force and sphere deformation for the case of linear elasticity is given by the equations (2)–(4) in Tatara [8]:

$$\delta = \frac{F}{E}\left(\frac{3\left(1-\nu^2\right)}{4a} - \frac{c}{\pi}\right) \tag{2}$$

$$a^3 = \frac{3\left(1-\nu^2\right)RF}{4E} \tag{3}$$

$$c = \frac{2(1+\nu)R^2}{\left(a^2+4R^2\right)^{\frac{3}{2}}} + \frac{1-\nu^2}{\sqrt{a^2+4R^2}} \tag{4}$$

where a is the radius of the circular contact area.

The normal force, F, was plotted against the total axial strain applied on the granule in Figure 3. Overall, the FEA force data is in very good agreement with Tatara's analytical solution. The disparity between the two stabilises at around 2% at axial strains beyond 0.5%, which for the purposes of verification is considered acceptable. On the contrary, the magnitude of the disparity between the FEA force data and Hertz increases monotonically with strain: from 3.8% at 1% axial strain to 8.0% at 3% axial strain to 11.0% at 5% axial strain.

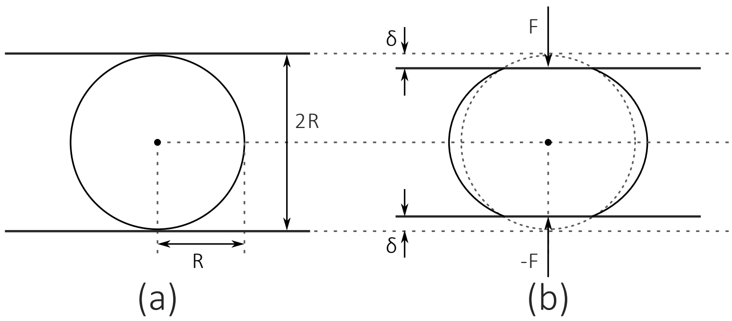


Figure 1: Schematic showing a single sphere with radius R (a) before and (b) after uniaxial compression between two rigid plates, with F being the normal force applied on the granule by the rigid plates and δ being the sphere deformation. Adapted from Constandinou and Hanley [5].

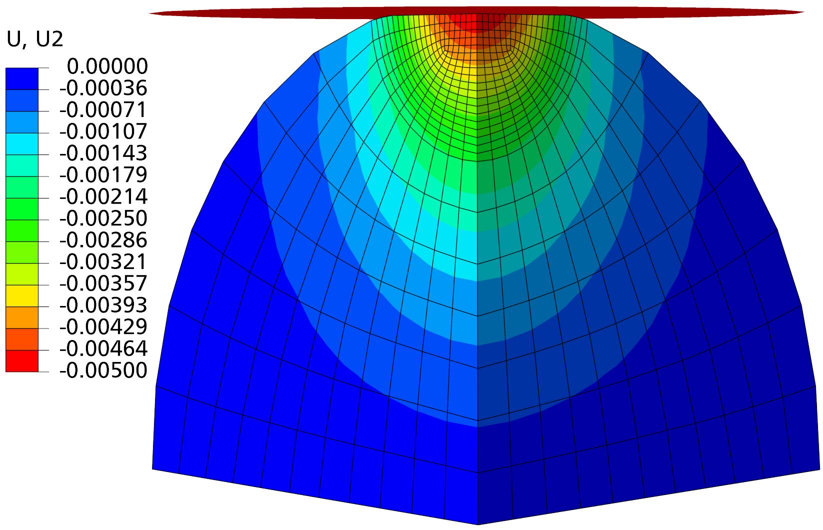


Figure 2: Octant of the sphere simulated in Abaqus FEA at an axial strain of 5%. The contours represent the y-axis displacement (perpendicular to the plate) measured in mm.

2.2 Parametric Study – Uniaxial compression of two-sphere rods

Having established the capacity of FEM to reliably predict the contact force for uniaxial compression of a single sphere, a parametric study for the uniaxial compression of two-sphere rods with varying sphere overlaps based on distance was conducted. An overlap of 0% corresponds to two spheres in touching contact; an overlap of 100% would correspond to both spheres occupying the same space, represented as a single sphere in FEM. Both spheres in a rod had the same radius. The parametric study consisted of 21 quasi-static compression simulations of two-sphere rods with sphere overlaps ranging from 0–100%. The two-sphere rods were compressed along their length. A number of configurations of two-sphere rods are shown schematically in Figure 4(b). The same material parameters and meshing procedures were used as for the single sphere case. Furthermore, the same data were used which consisted of the displacement of the plate from its initial position, δ, and the reaction force acting on the plate due to compression, F.

3 Results and Discussion

The results of the parametric study are summarised in the contour plot shown in Figure 4(a). The x-axis indicates the axial strain applied on the two-sphere rods, while the y-axis indicates the percentage sphere overlap within the two-sphere rods based on distance. The contours indicate the relative errors between the FEA results and the Hertzian contact model. A Hertzian model was used for comparison as, unlike Tatara [8], this is commonly used in DEM. The FEA model is taken as the basis for the relative errors; therefore a positive error is when Hertz is overpredicting the normal contact force and a negative error is when Hertz is underpredicting the normal contact force.

The axial strain percentages are only plotted from 0.1 to 5%. That's because at 0–0.1%

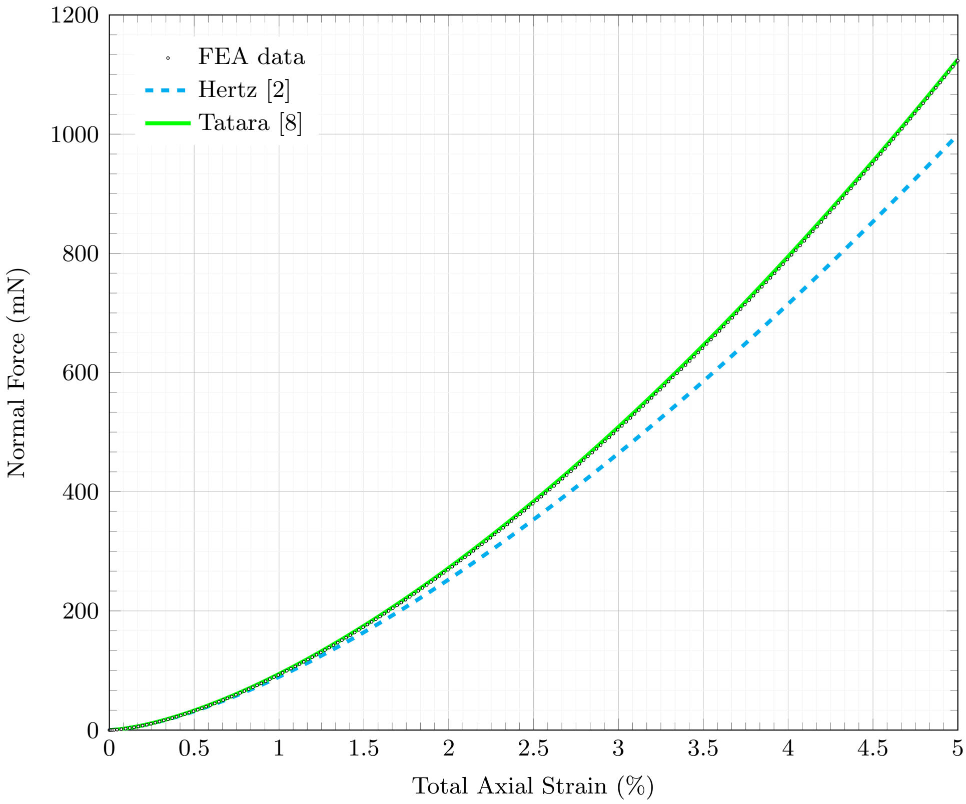


Figure 3: Normal force, F, against axial strain of a single sphere subjected to uniaxial compression in FEA, compared with analytical curves of Hertz [2] and Tatara [8].

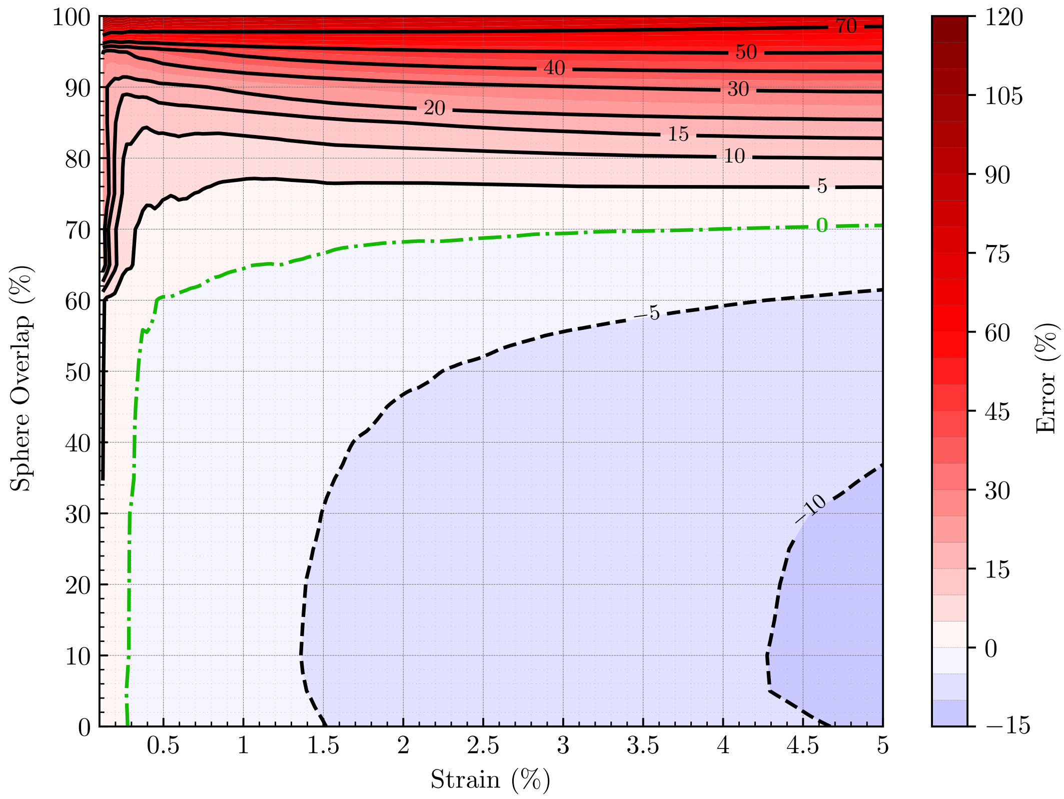
strains the relative errors can be unreliable because of the small denominator in the calculation. An additional schematic is included in Figure 4(b) to aid in the contour plot's comprehension.

For the rods with a sphere overlap less than 70%, Hertz generally underpredicts the contact force applied. At low deformations up to about 1.5% strain Hertz has a good agreement with the FEA results. The relative errors remain less than 5%. As the strain increases, the deviation between the FEA model and Hertz force increases monotonically in magnitude. As for the rods with a sphere overlap greater than 70%, Hertz overpredicts the normal contact forces. However, the strain ceases to be the main factor and instead the sphere overlap becomes the main driver of this deviation. As a result of this dependency change, the two-sphere rod with a sphere overlap of 70% shows a very good agreement with the Hertzian contact model even at high strains.

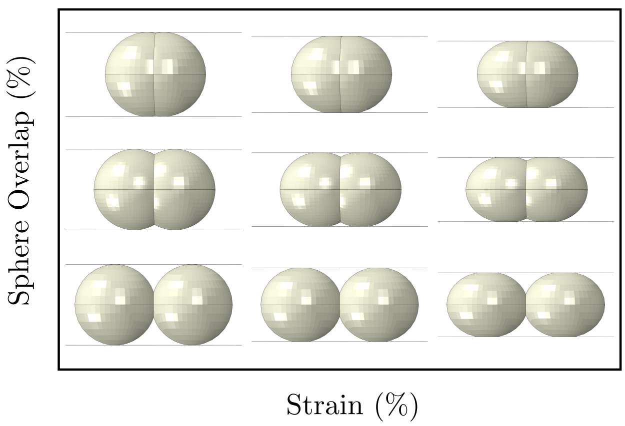
4 Conclusions and Future Research

The authors have successfully quantified to a reasonable extent the errors present in a multi-spherical particle DEM simulation utilising the Hertzian contact model. This can serve as a guide for DEM simulators and assist them in estimating the error bounds for their simulations.

Alternative contact models are needed for modelling non-spherical particles in DEM, such as Kumar et al. [11] for spherocylinders. Its suitability at non-infinitesimal strains is currently



(a) Two-sphere rod contour plot



(b) Compression Schematic

Figure 4: (a) Comparison of the force response of a two-sphere rod at various sphere overlaps obtained through the FEA model against the one obtained through the Hertzian contact model. The contours are indicating the relative errors present, while the signs of the errors represent whether Hertz is overpredicting (positive error) or underpredicting (negative error) the contact force based on the FEA results.
(b) Schematic representation of various two-sphere rod configurations based on spatial location within the contour plot. Deformations have been exaggerated to enhance clarity of representation.

being investigated by the authors.

Future research will focus on the other source of error identified in multi-spherical DEM simulations arising from the shape discrepancy between the actual particle and its approximation. This will involve similar quasi-static compressions of perfect spherocylinders and multi-spherical rods composed of more spheres, as well as some dynamic collisions of the two types of particles taking place at various angles.

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