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# Towards a mechanistic contact model for elastoplastic particles at high relative densities

Göran Frenning [1]

*Department of Pharmacy, Uppsala University, P.O. Box 580, SE-751 23 Uppsala, Sweden*

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ABSTRACT

Triaxial compression of elastoplastic particles was studied with numerical and analytical methods in order to develop a mechanistic model for their interactions at high relative densities. The introduction of an equivalent particle radius that accounted for the elastic volumetric deformation enabled an almost perfect reduction of the results obtained for elastoplastic particles to those obtained for rigid, perfectly plastic ones. This, in turn, made possible a simplified yet mechanistic analytical analysis of the particle response in terms of the contact area, pressure and force. The developed model exhibited a good agreement with the numerical results, especially for intermediate and large strains, and hence laid the foundations for the development of mechanistic contact models suitable for simulations of granular materials at high relative densities with the Discrete Element Method (DEM).


## 1. Introduction

The discrete element method (DEM), developed by Cundall and Strack [1], has established itself as the *de facto* standard technique for micromechanical simulations of granular systems. However, the DEM cannot in its current form reliably address issues related to compaction of granular materials at high relative densities, because of its inherent assumption of independent contacts and the lack of appropriate contact models. It has been recognised for quite some time that contacts can no longer be considered independent for relative densities exceeding about 0.85–0.90 for nonporous monodisperse spherical particles [2,3] and it has recently been claimed that effects of contact impingement cannot be neglected at relative densities as low as 0.7 if a particle-scale analysis is aimed at [4]. Hence, local models such as the ones proposed by Storåkers et al. [5], Thornton and Ning [6], Vu-Quoc and Zhang [7] and Brake [8] are not adequate in this range.

More elaborate methods can be used to circumvent these issues, such as the combined finite/discrete element method (FEM/DEM) [9–11], also referred to as the multiparticle finite element method (MPFEM) [12,13,4] or the meshed discrete element method (MDEM) [14]. The FEM/DEM is able to provide highly valuable results for small systems, but is unpractical for large-scale simulations due to its prohibitive computational cost. Hence, the DEM represents the most viable compromise between efficiency and accuracy, but new contact models are needed.

Significant progress towards the development of contact models valid at high relative densities has been made by Harthong et al. [4,14] who have presented a semi-empirical model for the behaviour of plastic particles. In this approach, the standard overlap-based contact force was augmented by a density-dependent singular term that accounted for plastic incompressibility, using a local relative density inferred from a Voronoi tessellation [15,16]. In an attempt to account for the constraint imposed by plastic incompressibility in an average sense, keeping the notion of independent contacts, a maximal plastic overlap was introduced in the truncated Hertzian contact model [6,17]. The maximal plastic overlap was inferred from a regular particle packing and represented the junction where the ability of plastic particle deformation was exhausted [17]. A more fundamental model, albeit restricted to contact between elastic spheres, has been proposed by Gonzalez and Cuitino [18]. Invoking the principle of superposition, as appropriate for linear elasticity, the overall particle deformation was expressed as a sum of the deformations resulting from each individual contact. Comparison with FEM/DEM results indicated that a superior representation of the particle responses under compression was obtained when contact dependence was properly accounted for. As a first step towards a mechanistic model for the interaction between plastically deforming particles under confined conditions, a geometrical analysis of the deformed particle shape was made in terms of a truncated sphere whose radius increased to accommodate the displaced material [19], building on the work by Fischmeister and Arzt [2] and Montes et al. [20].

Although the truncated sphere model [19] exhibited a satisfactory agreement with numerical results for different triaxial

*E-mail address:* goran.frenning@farmaci.uu.se
[1] Tel.: +46 18 471 43 75; fax: +46 18 471 42 23.

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loadings, it cannot describe the response at large volumetric strains, for two reasons. First, contact impingement invalidates the area determination, since the contacts will cease to be circular at large strains. Second, spatial confinement produces a mean contact pressures that exceeds the hardness, a process referred to as 'geometrical hardening' by Sundström and Fischmeister [21]. In order to address these issues in an as simple geometric context as possible, this work focuses on hydrostatic triaxial compression and develops a simplified mechanistic model for the particle response. In the light of previous work in the field, the adopted hydrostatic triaxial loading is expected to provide insights that can be generalised to more general loading conditions, because the crossover between a stage dominated by plastic deformation and a stage dominated by elastic deformation appears to be largely controlled by the degree of confinement, as quantified by a Voronoi tessellation [2,4,14]. Such extensions to more general loading conditions are discussed.

## 2. Numerical analysis

As in [19], the finite element method (FEM) was used to study the mechanical response of single particles under triaxial loadings. The onset of plastic flow was governed by the classical von Mises yield function, with yield stress $\sigma_y$ and no hardening. The elastic response was derived from a free-energy function of the compressible neo-Hookean type, containing two material constants that can be calculated from the Young's modulus $E$ and Poisson's ratio $\nu$. Simulations were performed for initially spherical particles with radius $R_{p0} = 0.5$ mm. The Young's modulus $E$ was kept fixed at 10 GPa, and four different values of Poisson's ratio were used ($\nu = 0.3, 0.4, 0.45$ and $0.49$), corresponding to bulk moduli $\kappa = E/[3(1-2\nu)]$ of 8.33, 16.67, 33.33 and 166.7 GPa. Likewise, two different yield stresses were assumed (100 and 200 MPa), corresponding to $E/\sigma_y$ ratios of 100 and 50. The particles were loaded along the $x$, $y$ and $z$ directions, using constant loading rates. A sliding boundary condition was used between the particle and the confining walls, i.e., the friction coefficient was put equal to zero.

Due to the reflection symmetries in the $x$, $y$ and $z$ planes, one octant of the particle was discretised by using about 41 500 hexahedral finite elements. Specifically, the total displacement version of the physically stabilised hexahedral element proposed by Puso [22] was adopted. This element eliminates shear and volumetric locking and is also relatively accurate for coarse meshes. Moreover, as shown by Reese et al. [23,24], elements that exhibit small mesh-distortion sensitivity may be devised by evaluating the stabilisation stiffness on the equivalent parallelepiped rather than on the element itself, which in effect means that the hourglass vectors $\mathbf{h}_i$ are substituted for the stabilization vectors $\boldsymbol{\gamma}_i$ (refer to [22] for the explicit definitions). Since numerical tests confirmed that the substitution of $\mathbf{h}_i$ for $\boldsymbol{\gamma}_i$ in the Puso element indeed significantly reduced its mesh-distortion sensitivity [10], this slightly modified element was used in the simulations. For ease of implementation, an explicit solution scheme was employed, with sufficient damping so that quasi-equilibrium was maintained.

## 3. Theory

During confined conditions in general and hydrostatic compression in particular, elastic deformation is expected to be primarily manifested as a volume reduction of the particle. To decouple the elastic and plastic deformation, it proves convenient to introduce an equivalent particle radius $R_{eq}$ such that the current particle volume $V_p$ can be expressed as

$$V_p = \frac{4\pi R_{eq}^3}{3}. \tag{1}$$

The usefulness of this definition stems from the fact that the equivalent particle radius $R_{eq}$ can be used instead of the initial particle radius $R_{p0}$ in a geometric analysis of the particle shape.

To estimate the magnitude of the elastic volume reduction, the average pressure in the particle is expressed in two different ways. First, the average stress $\boldsymbol{\sigma}$ can be calculated as a sum over the $n$ contacts [25],

$$\boldsymbol{\sigma} = \frac{1}{V_p}\sum_{i=1}^{n} \mathbf{F}_i \otimes \mathbf{r}_i, \tag{2}$$

where $\mathbf{F}_i \otimes \mathbf{r}_i$ denotes the tensor product between the force $\mathbf{F}_i$ on contact $i$ and the radius vector $\mathbf{r}_i$ pointing from the particle centre to the contact point. For hydrostatic triaxial compression with $n=6$, $\mathbf{r}_i = r\hat{r}_i$ and $\mathbf{F}_i = -F\hat{r}_i$, where $\hat{r}_i$ is an appropriate unit vector, the average pressure $P$ becomes

$$P = -\frac{1}{3}\mathbf{tr}\boldsymbol{\sigma} = \frac{2rF}{V_p} = \frac{3\bar{r}\bar{F}}{2\pi}, \tag{3}$$

where the last equality follows from the definition (1) once the scaled quantities $\bar{r} = r/R_{eq}$ and $\bar{F} = F/R_{eq}^2$ have been introduced. Second, using the definition of the bulk modulus $\kappa$, the average pressure can be expressed as

$$P = \kappa\left(1 - \frac{V_p}{V_{p0}}\right) = \kappa\left(1 - \frac{R_{eq}^3}{R_{p0}^3}\right), \tag{4}$$

where $V_{p0} = 4\pi R_{p0}^3/3$ is the initial particle volume and where the second equality follows from the definition (1). Combining Eqs. (3) and (4), one obtains

$$R_{eq} = R_{p0}\left(1 - \frac{3\bar{r}\bar{F}}{2\pi\kappa}\right)^{1/3}. \tag{5}$$

Assuming that the particle shape for small to intermediate strains can be described as a truncated sphere of radius $R$ (Fig. 1a), the particle volume can be determined as the difference between the volume of the sphere ($4\pi R^3/3$) and the volume of 6 spherical caps [each of volume $(\pi/3)(2R^3 - 3R^2 r + r^3)$], i.e.,

$$V_p = \frac{8\pi}{3}\left(-R^3 + \frac{9}{4}R^2 r - \frac{3}{4}r^3\right). \tag{6}$$

In the light of the definition (1) this becomes

$$\bar{R}^3 - \frac{9\bar{r}}{4}\bar{R}^2 + \frac{3\bar{r}^3}{4} + \frac{1}{2} = 0 \tag{7}$$

where $\bar{R} = R/R_{eq}$. The solution to this cubic equation can be expressed as

$$\bar{R} = A\left\{2\cos\left[\frac{\arccos(B/A^3 - 1) + \pi}{3}\right] + 1\right\} \tag{8}$$

where $A = 3\bar{r}/4$ and $B = 3\bar{r}^3/8 + 1/4$. In the absence of non-idealities (see below), contact impingement would occur when $\bar{r} = \bar{r}_1 = \bar{R}/\sqrt{2}$ (Fig. 1b) and Eq. 7 implies that

$$\bar{r}_1 = \frac{1}{(15/2 - 4\sqrt{2})^{1/3}} \approx 0.816. \tag{9}$$

Once contact impingement occurs, the free particle surface will be described as sphere with radius $\sqrt{2}(r-s)$, where $s$ is half the length of the straight segment of the contact boundary (Fig. 1c). Hence the particle volume can be expressed as the difference between the volume of a cube with side-length $2r$ ($8r^3$) and the volume of 8 corners [each of volume $c(r-s)^3$, where $c$ is an as yet