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## Study of cold powder compaction by using the discrete element method

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#### ABSTRACT

The discrete element method (DEM), based on a soft-sphere approach, is commonly used to simulate powder compaction. With these simulations a new macroscopic constitutive relation can be formulated. It is able to de-scribe accurately the constitutive material of powders during the cold compaction process. However, the force-law used in the classical DEM formulation does not reproduce correctly the stress evolution during the high density compaction of powder. To overcome this limitation at a relative density of about 0.85, the high density model is used. This contact model can reproduce incompressibility effects in granular media by implementing the local solid fraction into the DEM software, using Voronoi cells. The first DEM simulations using the open-source YADE software show a fairly good agreement with the multi-particle finite element simulations and experimental results.

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#### 1. Introduction

Powder metallurgy has long been an attractive process technology for both advanced and conventional materials. In a forming operation, powder is consolidated into a desired shape, normally by applying pressure. After forming, the green body (i.e., the compacted body) is sintered so that the mechanical resistance of the final component is effective [2]. Using powder compaction can save both time and money in the manufacture of mechanical parts in serial production. One of the major advantages is that near net shape parts produced by this process need little or no machining. Another significant advantage is the possibility to design the material properties by mixing different powder materials so that the final product achieves a specifically desired mechanical behavior. This results in a very high density (i.e., compact density greater than 0.9) conducive to forming a more homogeneous material suitable for high strength applications.

But in the powder compaction process, plasticity and elasticity phenomena, internal friction of porous medium and frictional effects between the die walls may induce inhomogeneous distributions of density and residual stress [3]. As a consequence, cracks appear into the compacted zone during the pressing process and the mechanical behavior of that part is difficult to predict [16]. To understand the complicated behavior of the powders, industrials have performed expensive trial and error procedures. With this in mind, numerical

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methods can be considered as a cheap and easy solution to help the prediction of the product properties, but the two numerical approaches known based on the finite element method (FEM) [15,21] and the discrete element method (DEM) [7,8] reproduce these phenomena with some difficulties. These obstacles are mainly due to the nonlinear material behavior during the pressing step [6].

Nevertheless, understanding and predicting the mechanical behavior of the final component can be done by the micro-mechanic simulation with adequate phenomenological models. These models may mimic the compaction process [9], because the DEM can give interesting insight on the different physical phenomena present during the early stage of powder compaction [16,22].

In this paper, we use a new micro-mechanic model to perform discrete numerical simulations of powder compaction up to a density equal to 0.95. In Section 2, we present the existing and new discrete models which are developed to simulate the powder process. Then in Section 3, the simulations of isostatic and die compaction of random packings are performed with both the existing and the new discrete models. The results are then compared to experimental results or the multi-particle finite element method (MPFEM) simulations [4,17].

#### 2. Discrete models

In DEM, the motion of each particle is resolved by using an explicit integration method from Newton's second law [20]. The force and moment that act on each particle result from the interaction forces with their neighboring particles and these forces are numerically computed by means of a force-law (i.e. an explicit relation between the force components and the local parameters). The DEM can easily

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simulate complex constitutive mechanical behaviors of granular materials with force-laws which integrate physical parameters, due to the discrete character of the sample. In this section, we present the force-laws commonly used to model the powder compaction and we introduce a new contact model (so called high density model) developed to simulate the compaction up to a high density value. Only material parameters are required for these models and no calibration is needed.

#### 2.1. Existing models

In the simulations of compaction based on DEM, the powder is often represented by elastic-plastic spheres. The elastic part of the contact force is generally given by the Hertz contact law that expresses the normal elastic force  $F_{ij}^e$  between two spheres i and j as a function of their overlap  $h_{ij}$ . This force-law reads:

$$F_{ij}^{e} = \frac{4}{3} \left( \frac{1 - \nu_{i}^{2}}{E_{i}} + \frac{1 - \nu_{i}^{2}}{E_{j}} \right)^{-1} \sqrt{R_{ij}^{*}} h_{ij}^{\frac{3}{2}}, \tag{1}$$

where  $R_{ij}^* = (R_i R_j)/(R_i + R_j)$  is the reduced radius of the particle i and j,  $E_i$  and  $E_j$  are the Young's moduli of their constitutive materials, and  $v_i$  and  $v_j$  are their Poisson coefficients. During compaction, particles in contact deform irreversibly and thus the plastic deformation of the constitutive material of the particles must be taken into account. The plastic force-law of Storåkers is generally used for this purpose. In the limiting case of a rate-independent material, it is based on a rigid-plastic Von Mises-type material with strain-hardening defined as:

$$\sigma = \sigma_0 \varepsilon^{\frac{1}{m}},\tag{2}$$

where  $\sigma$  and  $\epsilon$  are respectively the uniaxial Von Mises equivalent stress and strain,  $\sigma_0$  and m are material constants. The force-law derived by Storåkers [19] gives the normal plastic force Fijp between the particles i and j as a function of the plastic parameters  $\sigma_0$  and m of the particles:

$$F_{ij}^{p} = \pi \sigma_{0} 2^{\frac{2m-3}{2m}} 3^{\frac{m-1}{m}} c(m)^{\frac{2m+1}{m}} R_{ij}^{*\frac{2m-1}{2m}} h_{ij}^{\frac{2m+1}{2m}}, \tag{3}$$

where  $c(m) = \sqrt{1.43e^{-\frac{0.97}{m}}}$  is related to the area of the contact zone. This plastic force-law has been derived from finite element analyses and Hill's theory on the indentation of a rigid sphere with a deformable plane [11].

Some authors have used Storåkers's model (see Eq. (3)) coupled with the Hertz contact (see Eq. (1)) to perform discrete element simulations of powder compaction [5]. Nevertheless, this approach is limited in density, because it assumes the mechanical and geometrical independence of the contacts. Hence particles are considered to have only local deformation in the contact zones applied. These are small compared to the particles' sizes, and far from each other, such that there is no influence of the neighboring contacts. In theory, this assumption limits the model validity to the cases where interferences between the contacts are negligible [18], but it is generally accepted that the model is valid up to a relative density (i.e. the ratio of the volumetric mass of the powder relative to the volumetric mass of the material of its particles) of about 0.85. The model presented in the following overcomes this limitation by taking into account the contact interferences by means of a definition of the local solid fraction.

#### 2.2. High density model

The high density compaction analysis must absolutely account for the influence on each contact force of all the contacts around the particles. In the proposed model, this influence of these neighboring contacts are considered in an indirect way by using the concept of Voronoi cell as suggested by Arzt [1]. When a weighted 3D Voronoi partition of the packing is performed, the sum of all cell volumes correspond to the packing volume and each powder particle (initially spherical) are surrounded by a Voronoi cell that contains its own solid fraction (see Fig. 1). It is thus easy to define from the weighted Voronoi partition, a local solid fraction associated with a particle i:

$$\rho i = \frac{4}{3} \frac{\pi R_i^3}{V_i},\tag{4}$$

where  $V_i$  is the volume of the Voronoi cell surrounding the particle i. It is interesting to note here that  $\rho_i = 1$  means that the volume of the cell is completely filled by the material originally contained in the particle i.

To derive a force-law for the discrete element simulation of high density compaction, Harthong et al. [10] introduced a solid fraction  $\rho_{ij}$  defined at the contact level between particles i and j. In our implementation and in a first approximation, we arbitrarily defined this parameter as the average solid fraction of the adjacent cells i and j:

$$\rho_{ij} = \frac{1}{2} \left( \rho_i + \rho_j \right). \tag{5}$$

From finite element simulations of isostatic compaction of a cubic unit cell containing one spherical particle (see Fig. 2), Harthong et al. attempt to identify a force-law able to reflect the elastoplastic flow of the particles. The initial solid fraction of the unit cell was  $\rho_0 = 0.52$ . The high density force-law gives the normal force  $F_{ij}$  between the particles i and j as a function of the parameters  $\sigma_0$  and m of the particles. It has been formulated in the case where both spheres are identical, with the same radius R:

$$F_{ij}(t + \Delta t) = F_{ij}(t) + 2\sigma_0 R S_{ij} \left( m, \frac{h_{ij}}{R}, \rho_{ij} \right) \Delta h_{ij}(t). \tag{6}$$

In this relation, the stiffness  $S_{ij}$  depends both on material and geometric parameters:

$$S_{ij} = \alpha_1(m)e^{\beta_1(m)\frac{hij}{R}} + \alpha_2(m)e^{-\beta_2\frac{hij}{R}} + \alpha_3(m)\frac{\left[\max(0,\rho_{ij}-\rho^0)\right]^2}{1-\rho_{ij}}, (7)$$

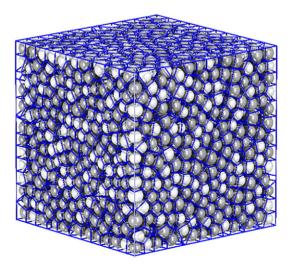


Fig. 1. Packing of 4000 spheres represented with the associated Voronoi cells.

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