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# Microscopic calibration of rolling friction to mimic particle shape effects in DEM

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## 1 INTRODUCTION

Much work has been done to characterize granular shape and to understand its influence on overall soil behavior. Thus, Wadell (Wadell 1932) introduced the concept of "sphericity" that quantifies how a particle differs from a sphere, in terms of surface area. Krumbein (Krumbein 1941) presents the first chart to visually estimate shape from the grain lengths ratios.

There is much evidence showing that particle shape is relevant for mechanical responses of soils. Andò (Andò 2013, Andò et al. 2012) tested in triaxial conditions different sands with shape ranging from very angular to rounded. Using Digital Image Correlation, he showed that angular sands exhibited a larger shear band thickness compared to rounded sands. Rorato (Rorato et al. 2019b) demonstrated that a rounded sand (Caicos ooids) exhibits higher grains rotations compared to an angular sand (Hostun sand).

In this work, we propose a new procedure for an optimal calibration of the DEM contact model parameters that is able to mimic the effect of particle shape without dramatically increase the computational time. In particular, our approach aims to (1) limit the number of free parameters requested, (2) respect the mechanical and kinematic triaxial responses of the sheared granular materials and (3) maintain low the computational time. The Particle Flow Code (*PFC3D*) developed by Itasca Consulting Group, Inc. (Itasca 2014) has been used in this work.

## 2 DESIGN AND ANALYSIS

The most widely used shape used in DEM is the sphere, because it allows straightforward and computationally efficient contact detection. Unfortunately, soil particles are not spheres. Some researchers has tried to tackle this challenge by introducing *non-spherical* elements, like clumps (*e.g.,* Katagiri et al. 2010, Lu & McDowell 2007), polyhedrons (*e.g.,* Elias 2013, Langston et al. 2013) or grain-shape-inspired particles (*e.g.,* Jerves et al. 2016, Kawamoto et al. 2018), at the price of increasing dramatically the complexity of the contact detection and computational time. Other researchers (Iwashita & Oda 1998, Jiang et al. 2005, Sakaguchi et al. 1993) have proposed the introduction of a resisting moment (*i.e.*, rolling resistance) into the contact law, beside normal and shear forces, in order to consider the influence of flat (*i.e.,* not punctual) contacts between real grains.

In this work, a simplified version - as implemented in the *PFC* software - of the Iwashita & Oda contact model has been used under the following assumptions:

(1) The *rolling stiffness* ($k_r$) is defined as the Iwashita & Oda's original contact model:

$$k_r = k_s R^2 \qquad (1)$$

where $k_s$ is the contact *shear stiffness* and $R$ the *effective radius* defined as

$$R=\frac{1}{R_1}+\frac{1}{R_2} \tag{2}$$

being $R_1$ and $R_2$ the radii of the two particles in contact.

(2) The moment-rotational contact law is implemented as an elastic-perfectly plastic model with the yielding moment ($M^*$) defined as:

$$M^* = \mu_r F_n \mathrm{R} \tag{3}$$

where $\mu_r$ is defined as *rolling friction coefficient* and $F_n$ is the normal contact force.

This paper exploits a novel approach to relate the particle shape with the rolling resistance applied at the contacts, extending the model that was originally proposed in (Rorato et al. 2018). In particular, it is hypothesized that the *degree of true sphericity* [1] ($\psi$), of one particle is univocally related with its *coefficient of rolling friction*, through a relation

$$\mu_r = F(\psi) = F\left(\frac{S_n}{S}\right) \tag{4}$$

valid for all the spherical particles participating in the DEM simulation. Therefore, if the statistical distribution of sphericity is known for one particular sand, it is possible to extract infinite values so that one measure of $\psi$ can be assigned to each sphere of the numerical specimen, and therefore the *rolling friction coefficients* can be distributed through all the discrete elements. The histograms of true sphericity for three different sands (Hostun, Caicos and Ticino sands), computed as in (Rorato et al. 2019a), are showed in Figure 1.

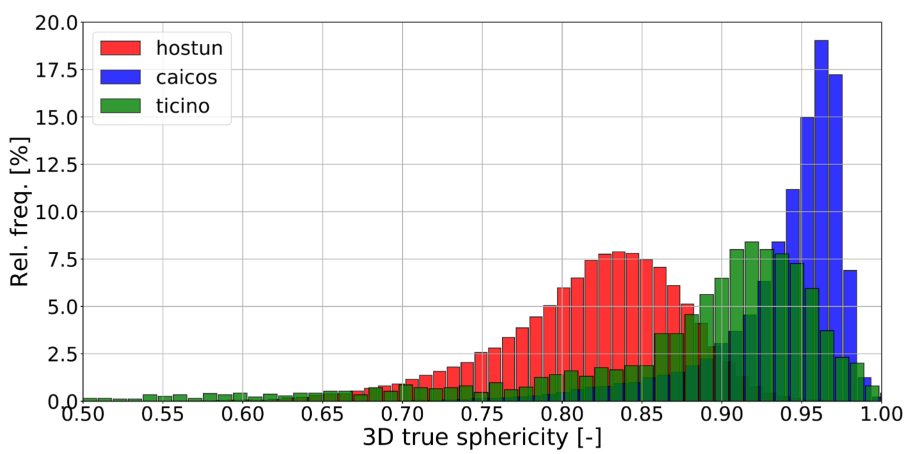



Figure 1. Statistical distributions of 3D true sphericity for Hostun, Caicos and Ticino sands.

The question then is what shape function $F(\psi)$ might take. We tried to find the equation of $F(\psi)$ that could best match the experimental triaxial tests performed on Hostun sand (specimen "HNEA01") and Caicos ooids (specimen "COEA01"). The calibration procedure here proposed aims to fit the conventional macro-mechanical responses together with kinematic measures. In particular, the histories of the cumulated grain rotations are known for each grain from the experiments have been measured and the particles rolling frictions have been adjusted to reproduce similar kinematic responses inside the shear bands of the numerical specimens. It is indeed well known from past DEM studies (Cheng et al. 2017, Estrada et al. 2008, Wensrich et al. 2014, Wensrich & Katterfeld 2012) that the same macroscopic friction angle can be obtained from

[1] Defined by Wadell (1932) as the ratio between the surface area ($S_n$) of the equivalent sphere (*i.e.,* same volume as the grain) and the surface area ($S$) of the particle.

several couples of *sliding friction coefficient* ($\mu$) and *rolling friction coefficient* ($\mu_r$). Both parameters contribute to the shear resistance of the numerical sample, and their influence is coupled. However, the rotational information - from the experimental measures of grains rotations - provides a unique numerical solution.

## 3 RESULTS AND DISCUSSION

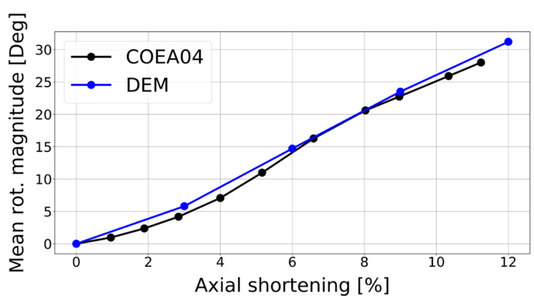
The equation of $F(\psi)$ has been finally chosen, after an iterative procedure, according to a power law written as

$$\mu_r = 0.1963(\psi)^{-8.982} \tag{5}$$

with an upper bound fixed at $\psi = 1$ (perfect sphere).

It is extensively shown in the full paper that it is able to reproduce the macro-mechanical responses (*i.e.,* stress-volumetric-strain) of HNEA01 and COEA04 sand specimens and the mean rotations inside the shear bands (*i.e.,* the kinematics at failure) throughout the execution of the triaxial test (Fig. 2).

Caicos (COEA04)
Mean rotations inside the shear band




Hostun (HNEA01)
Mean rotations inside the shear band

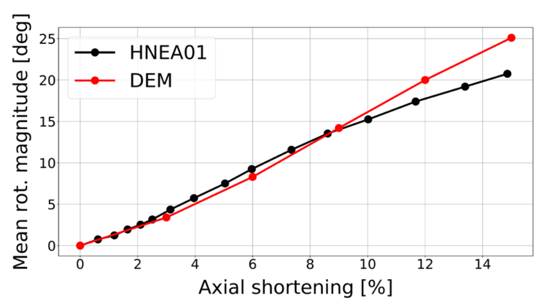



Figure 2. Histories of mean particle rotations for the grains located inside the shear bands for both the experimental and numerical samples, during triaxial shearing. The good fit ensures the kinematics at failure is respected.

The proposed approach has been then tested for validation in three different situations, achieving successful results, (1) at higher confining pressures, (2) testing a third type of sand (Ottawa sand) for which the statistical distribution of 3D sphericity was known and (3) testing a fourth type of sand (Ticino sand) for which the distribution of 3D sphericity was not known.

Regarding the third case, an innovative method is exploited to determine the statistical distribution of the *degree of true sphericity* (3D shape parameter) from 2D measures, as originally proposed by (Rorato et al. 2019a). In particular, a table scanner has been used to obtain an "oriented" projection of thousands of sand grains laying on their *plane of greatest stability*. The 2D outlines of all the particles thus obtained, can be then studies by image analysis techniques in order to extrapolate[2] the statistical distribution of $\psi$, and therefore of $\mu_r$, according to Eq. 5.

[2] It is known from (Rorato et al. 2019a) that the degree of true sphericity ($\psi$) is highly correlated with the *perimeter sphericity*, 2D shape parameter, after "oriented" particle projection (*i.e.,* perpendicularly to the minor particle length).

## 4 CONCLUSIONS

This paper presents an innovative technique to relate univocally the degree of true sphericity of each grain contained in a sand sample with the coefficient of rolling friction to apply to its numerical avatar of spherical shape. The main advantage of the proposed model is that it reduces the number of free parameters to set by trial-and-error procedures when performing DEM simulations, albeit respecting the grains kinematics at failure. Indeed, if the statistical distribution of sphericity is known, either from experiments either from the literature, the resisting rolling moment is entirely determined since all the parameters involved in the contact model are known or predictable.

Therefore, if the initial numerical sample reproduces the experimental void ratio (matched by adjusting the initial friction coefficient) and the PSD, the only crucial free parameter that must be determined for the shearing phase by trial-and-error procedures is the inter-particle sliding friction coefficient. Moreover, the contact detection remains economical and advanced algorithms are not required, maintaining low the computational time. This will open new frontiers to the use DEM for studying engineering applications at larger scales, especially in geotechnical problems in which the 3D particulate nature of the soil cannot be ignored.

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