IV International Conference on Particle-based Methods – Fundamentals and Applications
PARTICLES 2015
E. Oñate, M. Bischoff, D.R.J. Owen, P. Wriggers & T. Zohdi (Eds)

POWDER COMPACTION WITH POLYGONAL PARTICLES BUILT FROM RADIALLY EXTENDING ONE-DIMENSIONAL FRICTIONAL DEVICES

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Key words: Granular Materials, powder compaction, DEM, Contact Problems, Prandtl bodies

Abstract. Powder compaction is a major ingredient in a wide range of production techniques for objects of every day importance. Diverse applications – from pharmaceutical tablets to metallic and ceramic parts, where compaction is usually a part in the sintering process – are covered by current technology. The aim of cold compaction is to increase the relative density of the part.

Due to the granular nature of the powder material compaction is random process which requires careful mastering and comprehensive understanding. The experimental access to compaction processes, even as simple ones as uniaxial compaction, are limited. Therefore simulation of compaction processes offers the opportunity to improve understanding of powder compaction.

The Direct Element Method (DEM) simulates the powder as individual particles. These particles are distinct from each other and the forces applied to the entire powder are equilibrated by the contacting force between the particles. Usually, an explicit time integration, with or without considering dynamic effects, allows the particles to move and the powder to be compacted.

Especially for metallic powders the plastic deformation of individual particles plays an important role and has a perceptible influence up to the macroscopic scale of the whole part. This leads to efforts to formulate a DE method in which individual particles are discretized as distinct FE models. Yet, such approach is deemed too costly for the simulation entire parts.

Therefore a new approach for plastic particle deformation has been devised. The particles are simulated as 'hedgehogs' of one-dimensional frictional devices. The frictional devices form spikes that extend in a radial way from the center of the particle. The tips of the spikes are connected and the connections form the edges of the polygonal particles. The contacts between the particles are found by geometric means as intersections

of the spikes of one particle with the edges of the particle's contact partner. This indents the spike and its frictional device generates forces that act on the two particles. Multiple contacts between two particles are allowed and concave particles can be treated intrinsically.

Preliminary results indicate that this new approach to model plastic particles might bridge the gap between sufficiently realistic behaviour of the plastic particles and low computational effort. However, for now, the results are based on two-dimensional proof-of-concept simulations and, for the sake of simplicity, the springs in the spikes are linear and the friction is rate-independent and perfectly plastic. These model assumption already offer considerable liberties to tune the plastic behaviour of the particles to experimental results.

1 INTRODUCTION

In the simulation of the compaction of metal powder the defining factor is the inter-particle contact. Ideally it has to capture the entire physics of real-world particle interaction. It can be easily imagined that the contact involves elastic and plastic behaviour of the particles and both responses are likely to be highly non-linear.

A feasible concept is based on capturing of the elastic/plastic responses on the level of contact, as e.g. done by [1]. He uses rigid particles and contacts between them as separate entities. In fact the paradigm of object oriented programming promotes this view [2]. Whenever two, otherwise rigid particles come into contact a contact object between those two particles is constructed. This contact object stores all information relevant to the interaction between the particles. In particular, this could be information on the plastic deformation.

Obviously a problem arises once the powder changes its topology. Such topology changes are more present in uniaxial compaction than in isostatic compaction [3]. Supposing that two particular particles detach, the contact object is deleted and all information on contact is lost. Should these particles come into contact again, they would start over unaffected from the previous contact states. Even if the contact object for this particular pair of particles is stored for the case that the two particles should reconnect at a later time, the plastic deformation in the contact remains exclusive to these two particles. Should one of the two particles come into a contact with a third particle this would be a contact between two pristine particles, unaffected by the plastic deformation of the first particle.

This problem is usually solved by assuming that while new contacts are established, especially during the early phases of compaction when there is still rearrangement, the contacts on one particle are not mutually influencing each other [4]. This assumption will fail when e.g., later during the compaction, sliding planes occur in the powder [5]. Then the particles are already deformed to an extent that the different contacts acting on one particle are interacting while new contacts are established between already deformed particles.

The solution of this problem is obviously that the history of contacts has to remain at the level of the particles, and not at the level of the contacts. Outside the framework of DEM it is possible to eliminate the particles and to concentrate on the contacts alone. This can be achieved by introducting beam networks, see [6]. But inside the framework of DEM a particle is the central and only entity.

One possible approach is the Meshed Discrete Element Method (MDEM), where each particle is defined by a distinct finite element mesh [7, 8]. This approach offers the possibility for each particle to deform and remain in a deformed state after the resolution of a contact if plastic deformation occurred during the contact. Furthermore different contacts can interact at one particle. Depending on the mesh-size, the chosen material model, and the contact behaviour between the finite elements of two discrete meshed particles nearly every imaginable behaviour can be simulated.

However, there is a considerable drawback to the MDEM. Due to the required number of finite elements per particle and the contact search between the finite elements, the overall number of particles that currently can be simulated in a powder with the MDEM is counted in dozens rather than hundreds or even thousands. Therefore the MDEM is at the moment no feasible alternative to rigid particles whose plastic deformations are treated at the levels of the contacts.

This paper presents a novel approach that combines plastic deformation at the level of the particles at relatively modest computational costs. In this method polygonal particles are built from radially extending one-dimensional frictional devices or, for short, from hedgehog particles.

IN the following the concept of hedgehog particles is explained. Starting with a brief motivation for polygonal particles and it will be described how the frictional devices are arranged inside the particle. In the next steps the contacts between particles and the dynamics of the particles are described. In a closing section a proof-of-concept simulation is presented.

For the time being the hedgehog particles are limited to two dimensions. Thus one can focus on the main ingredients without the complexity of three-dimensional geometry. The aim of presenting a proof-of-concept simulation also supports the decision of remaining in two dimensions. The long term aim is to simulate powder compaction with topology changes and plastic deformation of the particles.

2 POLYGONAL PARTICLES BUILT FROM RADIALLY EXTENDING ONE-DIMENSIONAL FRICTIONAL DEVICES

2.1 Polygonal particles

The basic idea of deformable polygonal particles goes back to at least [3]. He and his co-workers observed experimentally that spherical copper particles deform to become polyhedra if compacted. Recently [9] revived the concept by formulating a repulsive force between rigid polygonal shapes. The force is formulated based on a potential in the overlapping area between two polygonal shapes. This presented work is based on these investigations and extends rigid polyhedra to deformable, polygonal shaped particles.

2.2 Perfectly plastic spring-friction-element

The spring-friction-elements form the spikes of the "hedgehog". They determine the deformation behaviour of the particle. The perfectly plastic spring-friction-element is also known as Prandtl-body. It can be implemented as a function that returns a force f for a prescribed displacement ϑ. Its internal state is described by the total deformation ϵ and the plastic deformation ϵ_p. The mechanical properties are determined by Young's modulus E, the yield stress σ and the flow variable γ. The reader is referred to the introductory chapter of [10] for more information. The geometrical properties of the spring-friction-element are described by the initial length $l^{(0)}$ and the area of the cross section A. Thus the force f can be expressed as $E\,A\,\epsilon$. The current length is $l = \epsilon\, l^{(0)}$ at any given time. The spring-friction element for the "hedgehog" particle includes in its implementation some additional checks to allow a force-less detachment from another particle during the resolution of a contact.

2.3 Hedgehog particles

The particle is defined as a "hedgehog" of n spring-friction-elements, each element forming a "spike". Figure 1 displays such a particle. The center of the particle is positioned at x_{part} and y_{part}. This point is common to all spikes of the particle. The whole particle can be rotated by an angle of ϕ_{part} against the x-axis.

Each spring-friction-element is positioned with its own angle ϕ_i against the unrotated position of the particle. The position angle of a spring-friction-element in the global coordinate frame is $\phi_{\text{part}} + \phi_i$. This facilitates the description of the tips of the spikes for a contact search, because the global coordinate frame is common for all particles. Each spring-friction-element has its own properties, like e.g. undeformed length $l^{(0)}$ and mechanical properties.

For the following contact search, all spikes must lie within the polygon of the particle. But the polygon does not have to be convex.

3 CONTACTS

The contact between two particles, as it is described in the following, will take place between the spike of a particle P_a and an edge of the particle P_b. For the special case of a spike-spike-contact a similar approach can be formulated. The methodology consists in finding an overlap ϑ between the edge and the spike. Then the spring-friction-element that is forming the spike is subjected to the overlap ϑ. The spike then returns a force as described in section 2.2. Finally this force is applied to the two particles that are in

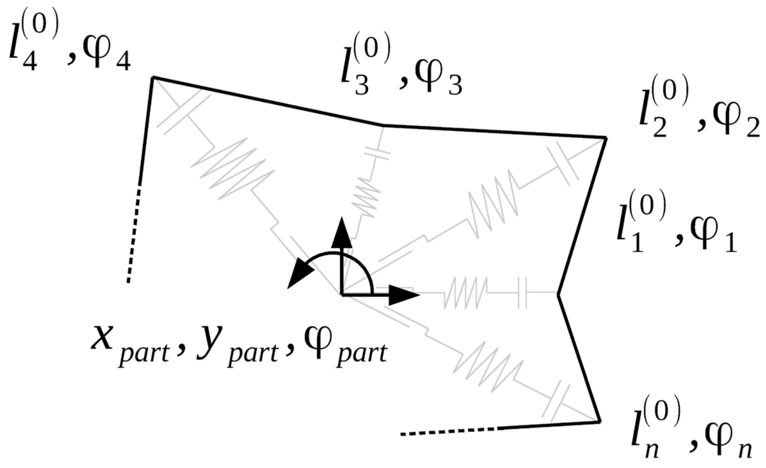

Figure 1: The prototypical, undeformed particle

contact.

3.1 Interparticle contact

As an example, the intersection is calculated between the i-th spike of P_a and the edge of P_b that spans between the spikes j and $j+1$. In order to compute possible overlaps with simple algebra, the spike and the edge are expressed as 2-tuples of points in the global coordinate frame, which is common for all particles.

This leads for the spike to

$$\vec{s} = \left\{ \begin{bmatrix} x_{\text{part}}^{(a)} + l_i^{(0)(a)} \cos\left(\phi_{\text{part}}^{(a)} + \phi_i^{(a)}\right) \\ y_{\text{part}}^{(a)} + l_i^{(0)(a)} \sin\left(\phi_{\text{part}}^{(a)} + \phi_i^{(a)}\right) \end{bmatrix} \quad , \quad \begin{bmatrix} x_{\text{part}}^{(a)} \\ y_{\text{part}}^{(a)} \end{bmatrix} \right\}, \tag{1}$$

It is important to note that the undeformed length of the spike is used. This allows a direct computation of the overlap ϑ.

For the 2-tuple of the edge the deformed length of the spikes is taken, because the particle P_b can be deformed. This yields

$$\vec{e} = \left\{ \begin{bmatrix} x_{\text{part}}^{(b)} + l_j^{(b)} \cos\left(\phi_{\text{part}}^{(b)} + \phi_j^{(b)}\right) \\ y_{\text{part}}^{(b)} + l_j^{(b)} \sin\left(\phi_{\text{part}}^{(b)} + \phi_j^{(b)}\right) \end{bmatrix} \quad , \quad \begin{bmatrix} x_{\text{part}}^{(b)} + l_{j+1}^{(b)} \cos\left(\phi_{\text{part}}^{(b)} + \phi_{j+1}^{(b)}\right) \\ y_{\text{part}}^{(b)} + l_{j+1}^{(b)} \sin\left(\phi_{\text{part}}^{(b)} + \phi_{j+1}^{(b)}\right) \end{bmatrix} \right\}. \tag{2}$$

The overlaps are calculated by solving

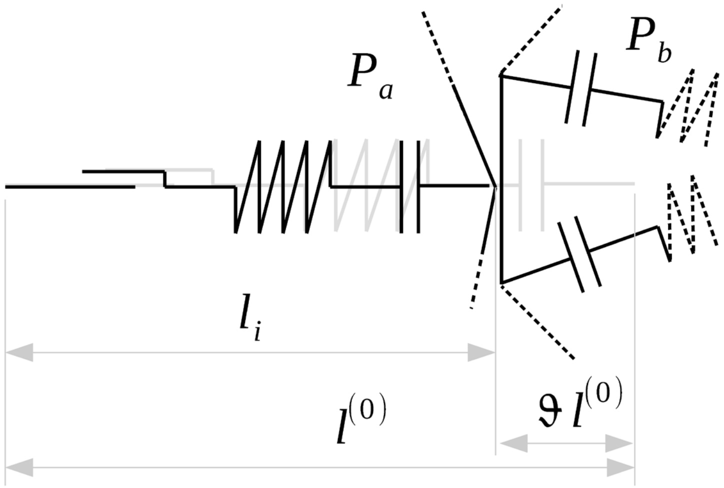

Figure 2: The prototypical spike-edge contact

$$\begin{bmatrix} \vec{s}_{2,x} - \vec{s}_{1,x} & \vec{e}_{1,x} - \vec{e}_{2,x} \\ \vec{s}_{2,y} - \vec{s}_{1,y} & \vec{e}_{1,y} - \vec{e}_{2,y} \end{bmatrix} \begin{bmatrix} \vartheta_a \\ \vartheta_b \end{bmatrix} = \begin{bmatrix} \vec{e}_{1,x} - \vec{s}_{1,x} \\ \vec{e}_{1,y} - \vec{s}_{1,y} \end{bmatrix} \tag{3}$$

for ϑ_a and ϑ_b.

If $0 < \vartheta_b < 1$ a contact might exist and ϑ_a is passed to the i-th spike to obtain a force f. This overlap is treated internally by the spring-friction-element. If the returned force is zero, the contact search is continued with other edges, spikes and particles, depending on the level the contact search algorithm is currently operating on. If, on the other hand, the force has a non-zero value $f \neq 0$, the spike i of P_a is indented accordingly in order to avoid a penetration into P_b. The force that is returned from the indentation of the spike is aligned along the direction of the spike

$$\vec{f} = f \begin{bmatrix} \cos\left(\phi^{(a)}_{\text{part}} + \phi^{(a)}_i\right) \\ \sin\left(\phi^{(a)}_{\text{part}} + \phi^{(a)}_i\right) \end{bmatrix} . \tag{4}$$

This force can be applied directly to P_a, because the spike passes through the center of the particle and no moment is generated.

For the particle P_b the force $\vec{f}$ is also applied to the center, but in addition a moment has to be calculated, because the force is applied at the intersection point of the undeformed spike and the edge. This intersection point is calculated as

$$\vec{i} = \begin{bmatrix} \vec{s}_{1,x} \\ \vec{s}_{1,y} \end{bmatrix} + \vartheta_a \begin{bmatrix} \vec{s}_{2,x} - \vec{s}_{1,x} \\ \vec{s}_{2,y} - \vec{s}_{1,y} \end{bmatrix} . \tag{5}$$

The generated moment is calculated as

$$m = \left\| \begin{bmatrix} \begin{bmatrix} x^{(b)}_{\text{part}} \\ z^{(b)}_{\text{part}} \end{bmatrix} - \vec{i} \\ 0 \end{bmatrix} \times \begin{bmatrix} \vec{f} \\ 0 \end{bmatrix} \right\| . \tag{6}$$

This moment is applied to P_b.

It should be noted, that, with this procedure, no spike of the particle P_b is indented. The reason for this is phenomenological. If a sharply pointed spike of a particle is pressed against the flat edge of another particle, it is safe to assume that the spike is indented, deformed and bent, while the edge receives only a local indentation mark, a scratch, so to speak, which does not affect the nearby spikes. This assumes similar materials.

3.2 The contact search algorithm

The above procedure is repeated for all n_a spikes of particle P_a with all n_b edges of particle P_b. Then the roles of P_a and P_b are inverted and the procedure is repeated for all n_b spikes of particle P_b with all n_a edges of particle P_a. During these calculations the deformed and undeformed lengths of the particles' spikes are frozen. The indentations of the spikes are only applied once the contact calculations are finished. This ensures that no particle is preferred and all overlaps that stem from the preceeding integration step are duly treated. Also, with this process, all overlaps are resolved.

On global level the possibilities of contacts between particles are checked with a primitive n^2 contact search and the longest spikes of each particle as radius of the enveloping circle. This approach is taken for the sake of simplicity and has to be abendoned for large particle assemblies.

4 PARTICLE DYNAMICS

The dynamics of the particles are adapted to the quasistatic nature of the compaction process. [11] argues that simulations including dynamical effects are better suited to rapid granular flows, like e.g. pouring, than for quasistatic processes, like e.g. compaction. [12] proposes an approach which is used for the simulation of Brownian motion. By eliminating the superposition of the underlying flow, the dynamic model can be formulated as

$$\vec{x}\,(t + \Delta t) = \vec{x}\,(t) + \boldsymbol{R}^{-1} \vec{F} \Delta t. \tag{7}$$

In this algorithm - based on an explicit Euler integration - the vector $\vec{x}$ combines the translational and rotational degrees of freedom of the particle, the vector $\vec{F}$ the forces acting on these three degrees of freedom and $\boldsymbol{R}$ is a resistance term, which can be different for each degree of freedom. The dynamic model neglects the inertia of the particles and is thus suitable for a quasistatic process.

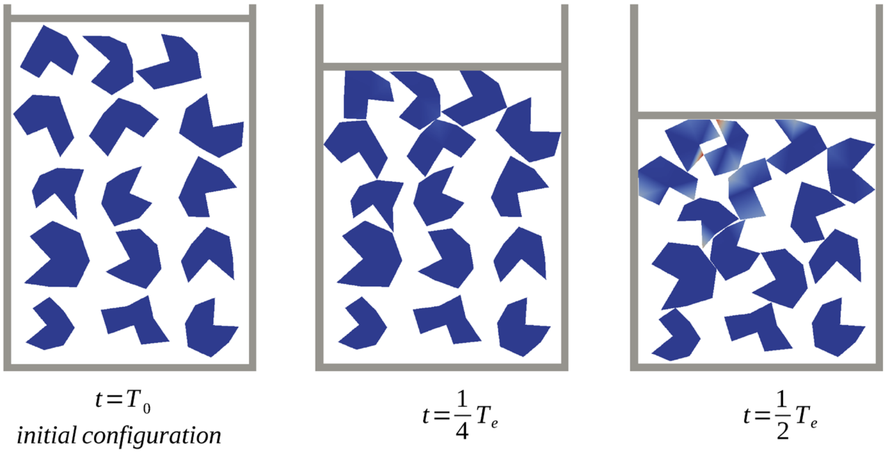

Figure 3: The initial configuration and the first two states of the proof-of-concept simulation

5 PROOF-OF-CONCEPT

The proof-of-concept simulation aims at establishing a multi-particle simulation. The main focus is set on contacts between multiple particles at the same time.

For the simulation 15 hedgehog particles are compressed uniaxially in a 2-dimensional die. The particles are randomly placed and do not contact each other at the beginning.

The figures 3 and 4 show the initial setup and four stages of compaction. The plastic deformation ϵ_p of the spikes is shown in colour.

The die consists of rigid walls. The contacts between particles and walls are treated the same way as the particle-particle contact, see section 3. In case of particle-wall contacts the walls are treated as edges and the particles' spikes deform due to contact with the wall. All contacts are considered as frictionless.

The forces exerted by particles on the walls are summed up. Figure 5 shows the force histories related to contact with the lower horizontal and the left vertical wall. The forces at the lower wall depict that the "powder" actually resists the compaction. The increase of the forces at the vertical wall shows that the powder produces a lateral pressure due to the compaction.

The force histories display a great deal of jittering. This jittering is introduced by the freezing mechanism during the contact search. If a spike comes into contact with an edge - which might also be a wall - the spike is indented. Then the particle is moved depending on the force returned from the spike. This can lead to a gap and thus the contact state is lost. If the amplitude of the force is large enough, the particle might move far enough, such that the contact is not reestablished for several time steps. Hence the force drops to

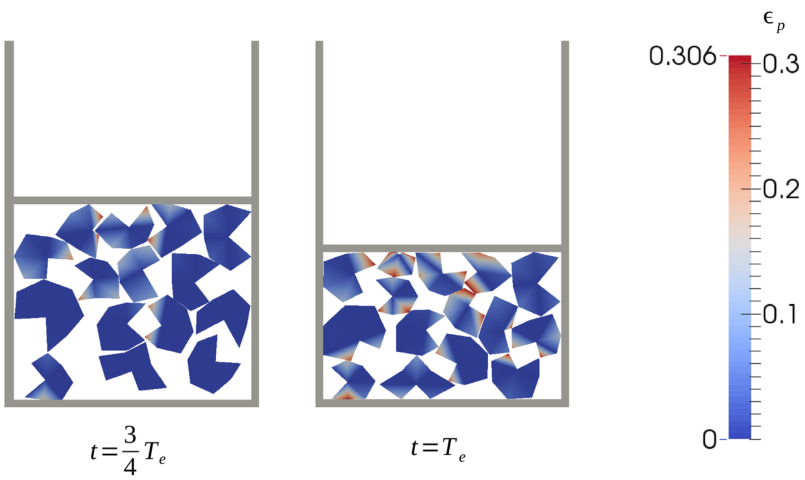

Figure 4: The last two states of the proof-of-concept simulation

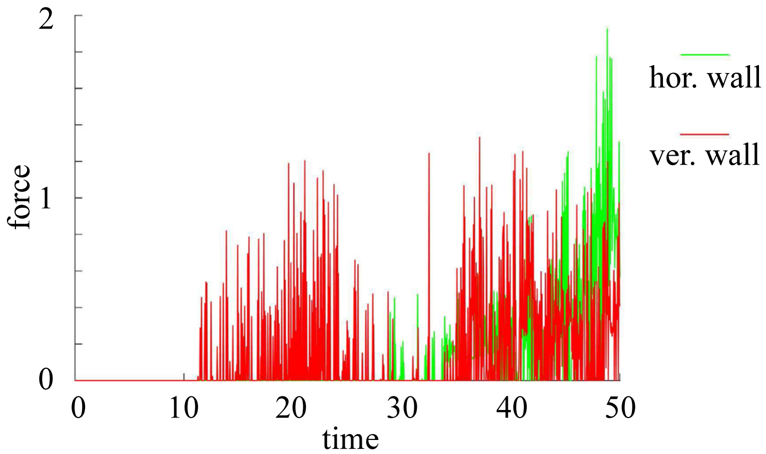

Figure 5: The vertical and horizontal forces on the wall

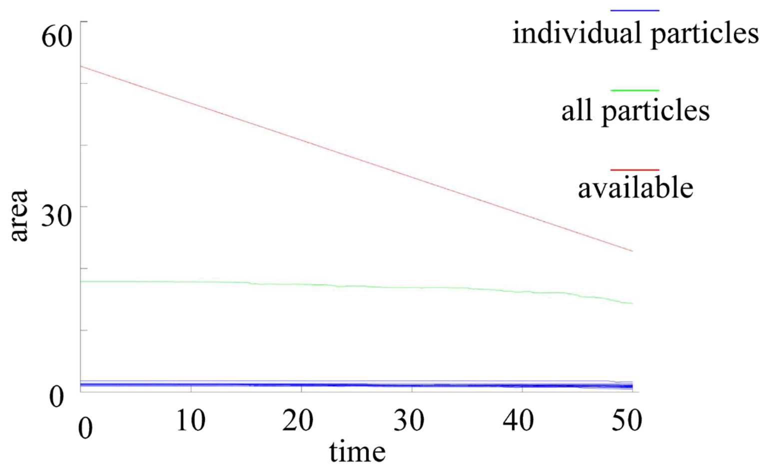

Figure 6: The areas involved

zero. If the contact partners reestablish their contact, the force returns to a high level. For the movement of particles, which happens generally in a smooth way, this can be neglected, but for the forces, that are recorded at every time-step, this jittering becomes very visible.

The transfer from vertical to horizontal forces proves that hedgehog particles can transfer a pressure. This transfer of a pressure is a feature of real powder compaction and is intuitively understandable. Naturally the curves of vertical and lateral stress obtained with this simulation do not match the ones obtained from experiments, like e.g. the ones performed by [13], because the hedgehog particles are not calibrated. But these curves could be applied to calibrate the properties of the hedgehog particles with respect to the experimental data. This would then enable the use of hedgehog particles for simulations with more realistic geometries than a simple die. However, this is beyond the aim of this proof-of-concept simulation.

6 CONCLUSION AND OUTLOOK

The presented work offers the hedgehog particle as a novel approach that combines the plastic deformation of particles with a probably acceptable computational cost. This should allow for a simulation of powder compaction with topology changes in which the particles retain their individual plastic deformation. The hedgehog particles consist of radially extending frictional devices and possess a quasi static behaviour. The contacts between the particles are defined as intersections of spikes with edges. This allows an intrinsic treatment of non-convex particles as long as the spikes remain inside the particle.

The hedgehog particles are subjected to a uniaxial compaction as a proof-of-concept simulation. This simulation demonstrates that the properties of the hedgehog particles can be calibrated against experiments.

Furthermore, the simulation illustrates the property of the particles of loss of area, which is not physical. This effect is shown in figure 6. If the area of the particles is linked by density to a mass, this effect would correspond to a loss of mass. This is neither desirable nor physically correct. Therefore an an isochoric condition - like $\det J = 1$ - has to bes introduced at particle level. If a spike gets indented, the other spikes should extend to compensate for the loss of area. This part is however ongoing research, because it is not easily determined how this isochoric condition could be formulated, especially considering that for some configurations all spikes of a particle could be indented at the same time. For this proof-of-concept simulation the loss of area is considered to be on the edge of being negligible on the powder level. However, for individual particles it can be rather significant and the loss of area is definitely an issue that has to be addressed during the further development of the hedgehog particles.

Also the absence of friction in the proof-of-concept simulation has to be considered as a major problem, because, as [14] argues, friction is the dominating mechanism in rather dense, static packing. Also, a slight friction might remedy the effects of resolving and reestablishing contacts which cause the observed jittering.

In the far future an extension of the concept to 3 dimensions should follow. There, the contacts would be the insertion of a spike of one particle with the triangle spanned between the tips of three spikes of the particle's contact partners. While the calculation of intersections in 3 dimensions is more complex.

In conclusion the prospect of simulating powder compaction with plastically deformable particles, that deform under high stress states and offer a modest computational effort, warrants the pursuit of the development of hedgehog particles in 2 and ultimately in 3 dimensions.

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