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EFFECT OF PARTICLE GEOMETRY ON THE RESULT OF DISCRETE ELEMENT SIMULATIONS USING POLYHEDRAL PARTICLES

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Abstract: Granular materials share a common characteristic; their intricate particle shapes. Due to this, a complex interaction arises between particles when they collide and fragment. Traditionally, it was common to use continuum methods, such as the finite element method (FEM), to reproduce the behaviour of these materials, even though these methods require complex constitutive models. In contrast, the Discrete Element Method (DEM) can model interacting solid bodies representing the behaviour of granular spherical)and polyhedral (non-spherical) particles, with focus on the micromechanics of particle interactions. A shortcoming of DEM is that no information about a stress/displacement field within a particle is generated during a simulation. Uniting DEM and FEM, the combined FEM/DEM presents a comprehensive approach considering the material as both continua and discontinua. Since the number of particles used in a simulation is limited by the computing power available, it is customary to use simplified geometries representing a particle. The simplest being a sphere, and any particle is seldom represented by more than a few hundred triangles. Irrespective of the method used, particle geometry has a potential to influence the outcome of a simulation. The effect of surface detail at various lengths of scale can affect the location of contact points, governing the applied forces. This paper summarizes the findings of an investigation of the influence of particle geometry (asperities) of polyhedral particles simulated by FEM/DEM. Both solution time and solution accuracy are considered, and results will be critically reviewed and recommendations will be given for practical use in simulations.

1 INTRODUCTION

In recent years, analysis of the behavior of brittle materials, such as concrete, rocks or granular materials, is receiving more attention. These brittle materials share common characteristics; their high complexity and heterogeneity, especially when they fragment from their original shape into smaller particles. Traditionally, it was common to use continuum methods (like the FEM) to reproduce the behavior of these materials, even though these methods require complex constitutive models, which contain a lot of parameters and variables that need to be appropriately tuned on a per-problem basis. The Discrete Element Method (DEM) (O'Sullivan, 2011), originally developed by Cundall and Strack (1979), in contrast to continuum methods, has been proven to be an irreplaceable and powerful tool for conducting analysis and modelling the behavior of spherical and polyhedral particle systems, which also focus on micromechanics of soil/rock particle interactions and displacements. In addition, there is another method named the Combined Finite-

Discrete Element Method (FEM/DEM) ((Munjiza et al. 1995, Munjiza 2004), which is a numerical solution that focuses on the analysis of problems for solids that are considered as both continua and discontinua. The FEM/DEM method of simulation is gaining popularity, because in addition to granular soil behaviour, processes like railway ballast behaviour or rockfalls can be modeled using it. Irrespective of the discontinuum method used, the main focus of this paper is the issue that to what extent does the level of geometric detail describing a particle, can influence the outcome of simulation or how much the presence of detail affect the length of simulation. Thus, the importance of this work is in evaluating the use of FEM/DEM to analyse collision of particles with different discretizations. Therefore, findings can serve as a reference for future research concerning simulation of soil, rock or general granular particle collisions to determine the sufficient geometric detail of particles that still leads to a reasonable simulation time, yet without losing the accuracy of simulation due to oversimplification of geometry.

2 BRIEF OVERVIEW OF CONTACT MECHANICS

During a DEM simulation, particles are interacting with each other, which requires the interaction analysis for those pairs that are in contact and those bodies that are potentially will get in contact (Johnson 1985). Then, it will be necessary to identify which actual particles are in contact and so the resulting forces acting on them can be determined. These two phases are defined as the ‘contact detection’ and ‘contact resolution’ phases during the simulation (Hogue 1998). The difficult part is to develop an algorithm for the contact detection stage, which is related to the complications on how to keep track those particles that are in contact and identify those particles will potentially get in contact. For a more detailed background and an overview of contact detection codes that are used in DEM simulation, the reader can be referred to the work by Munjiza (2004). For the contact resolution stage, the contact geometry and kinematics are required to be accurately determined, which will be aided by the implementation of a constitutive model and particle interpenetration assumptions. The calculation of contact forces, which represent the integral of stresses along contact surfaces, needs to consider two orthogonal parts (normal and tangential) with respect to the points of contact. These two forces always are represented by rheological models which comprise of springs, sliders and dashpots, and these rheological models are usually called as contact constitutive models (O'Sullivan 2011). For DEM simulations, it is common to simulate contacts as non-conforming and point contact assumption, due to the widely-used DEM models that employ a simplification of geometry such as spheres or disks. While in reality, the contacting situation is more likely to be a non-conforming contact initially, and will transform into a conforming contact with the yielding of asperities. Another important phenomenon during contact should be clarified, which is called as a traction that describes the surface pressure exerted along the contact surface as a result of contact forces. Symbols f_n and f_t are used to express the normal and tangential tractions independently, and the numerical resolution of contact forces in normal and tangential directions can be expressed by integration of these tractions over the contact area A_c as such show in Equation 1 (Matuttis and Chen 2014):

[1] $F_n = \int_{A_c} f_n dA \;\; F_t = \int_{A_c} f_t dA$

Considering that the changes of the shape and size for each particle will be a problem of finite strain elasticity, then the deformability of each particle is then represented by a continuum-based model. While the interaction among particles and the interaction between a container and particles is well-represented by a discontinuum-based model. Thus, in the simulation that uses this method deformability is represented by using continuum formulation (FEM) for particles, while discontinuum format (DEM) will be applied for the motion and interaction among particles. During the contact stage, one element is denoted as the contactor and the other element is denoted as the target (Munjiza 2004). During a contact, the overlapping area between the contactor and target is denoted as S, which is bounded by a boundary Γ. The detailed illustration can be seen in Figure 1, as:

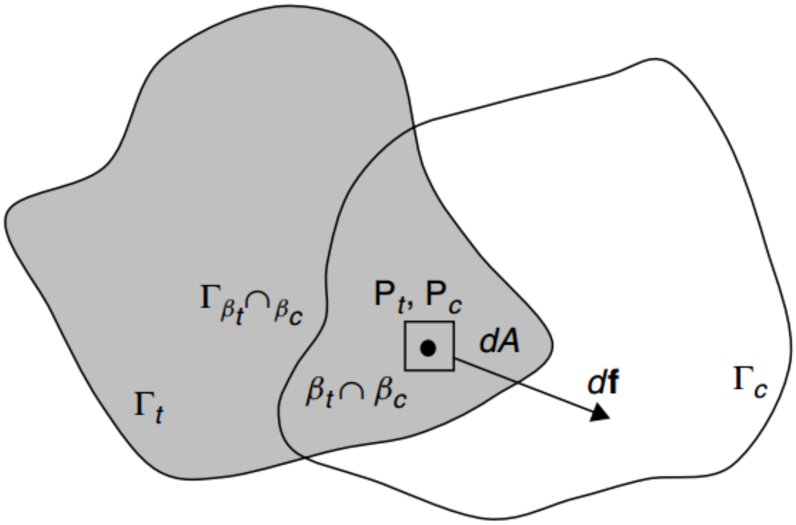

Figure 1: An illustration of infinitesimal overlap around points P_c and P_t, and the resultant contact force (Munjiza, 2004)

Thus, the total of infinitesimal contact force can be described as (Equation 2):

[2] $$df = E_p[grad\varphi_c(P_c) - grad\varphi_t(P_t)]dA$$

If we take the integral of Equation 2 over the overlapping area S between the contactor and target element, then the total of contact force yields, as seen in Equation 3,

[3] $$f = E_p \int_{S=\beta_t \cap \beta_c} [grad\varphi_c - grad\varphi_t]\, dA$$

which also equals to the integration over the boundary of the overlapping area Γ, as seen in Equation 4

[4] $$f = E_p \oint_{\Gamma_{\beta_t \cap \beta_c}} n\, \Gamma(\varphi_c - \varphi_t)dA$$

where n is the outward unit normal perpendicular to the boundary of the overlapping area, $\beta_t \cap \beta_c$ equals to the overlapping area S, as can be seen in Figure 1, and other parameters are the same as defined previously. In 3D, instead of considering the overlapping area S, the total contact force is calculated based on the overlapping volume V, as in Equation 5

[5] $f = E_p \int_V [grad\varphi_c - grad\varphi_t]\, dV$

and the potential is expressed over the tetrahedron, which can be illustrated in Figure 2

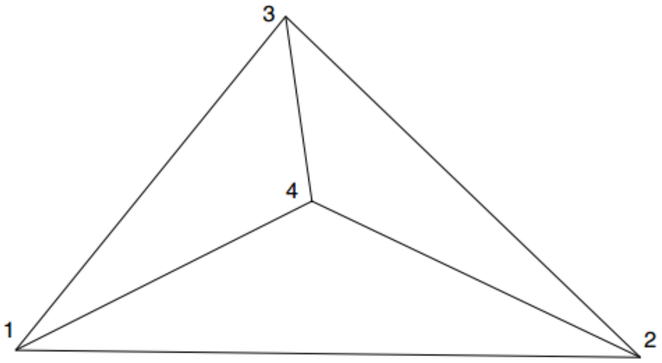

Figure 2: Potential definition over domain of a single tetrahedron (Munjiza 2004)

By using the tetrahedron model, the coordinates of the centroid of the tetrahedron can be calculated, which can provide us with four sub-tetrahedra. For any point p in the sub-tetrahedra (i – j – k – l), the potential φ is defined as:

[6] $\varphi(\mathbf{p}) = \mathrm{k}\left(\frac{V_{i-j-k-p}}{4V_{i-j-k-l}}\right)$

where k stands for the penalty parameter, $V_{i-j-k-l}$ is the volume of the tetrahedron i – j – k – l, while $V_{i-j-k-p}$ stands for the volume of the sub-tetrahedron i – j – k – p. For more detailed analysis about how to calculate the coordinates of the centroid of a tetrahedron, the reader can be referred to the work by Munjiza (2004).

3 PARTICLE COLLISION WITH A SOLID BLOCK

The simulation, using the Virtual Geoscience Workbench (Xiang and Munjiza 2008), was conducted focusing on a single particle with a given initial velocity colliding with a solid block under the influence of gravity. Although each simulation uses a single (but different) particle, there were a total of 200 simulations performed (one for each of the 50 particles, obtained using 3D scanning with a NextEngine scanner (NextEngine Inc. 2014), at a given mesh resolution, and 4 different resolutions per particle). For each simulation, several aspects of the collision results have been collected as a function of the change of the number of surface mesh elements (particles with 100, 250, 500 and 1000 surface mesh elements), which are: 1) resultant forces during collision for each particle; 2) comparison of impulses for different simulation results; 3) comparison of peak force for different simulation results; 4) comparison of CPU usage. Ideally, each resultant force versus time curve should overlap each other irrespective of particle mesh resolution. However, due to the differing geometric detail that affected initial contact and collision times, for some particles the collision and force behaviour was found to be different. Among the four aspects for each particle's simulation results, the first aspect is the main focus of the discussion and all potential reasons for non-overlapping resultant force curves will be explained; such as why the dispersion of certain curves in resultant force plot are different from other curves. While certain curves in the resultant force plot had a "tail" and certain curves were exhibiting asymmetry. All these points will be grouped and discussed below. As an example of the setup, Figure 3 shows a model of a single particle with different discretization resolutions, while Figure 4 shows a collision response which has the resultant forces overlapping.

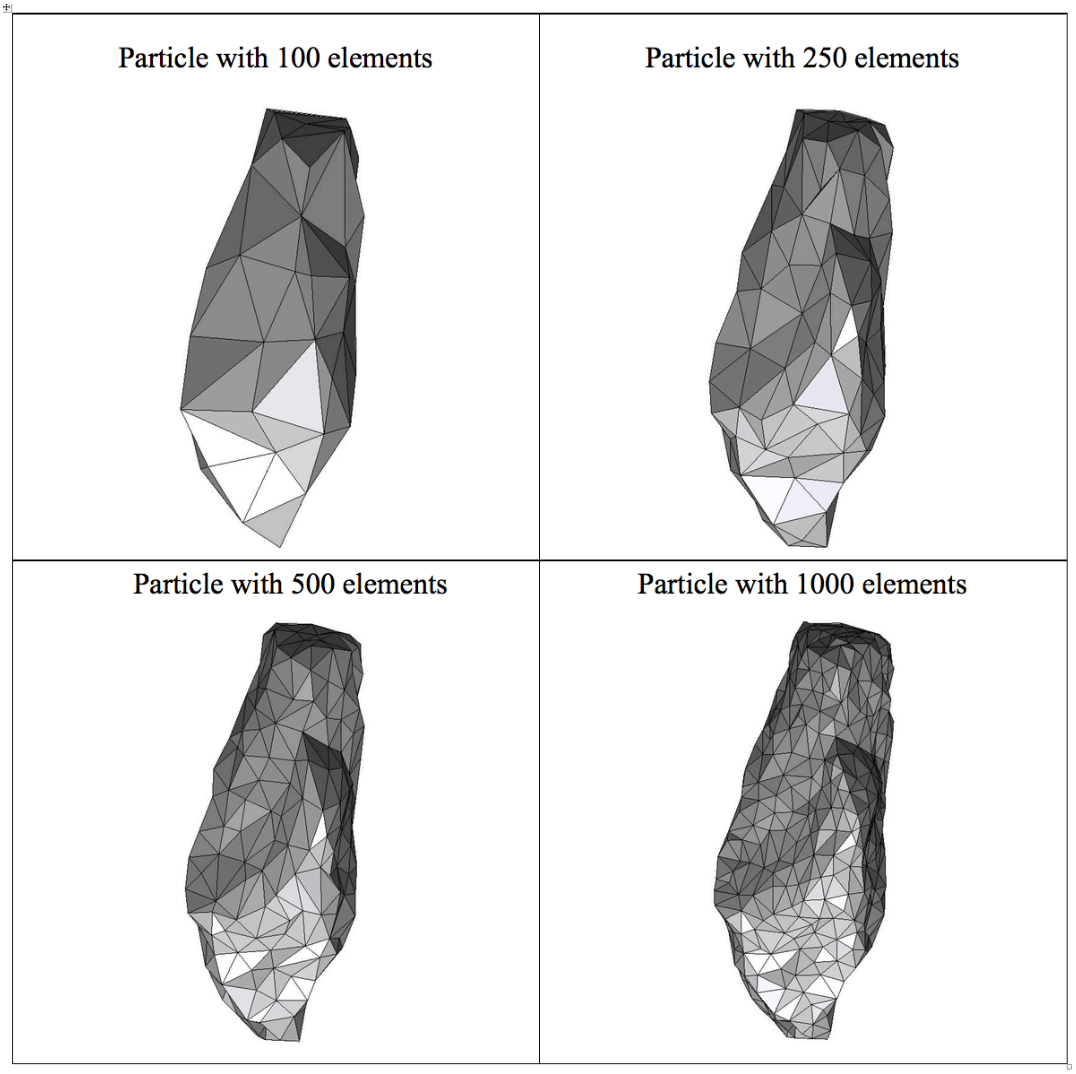

Figure 3: Different discretization resolutions of a particle

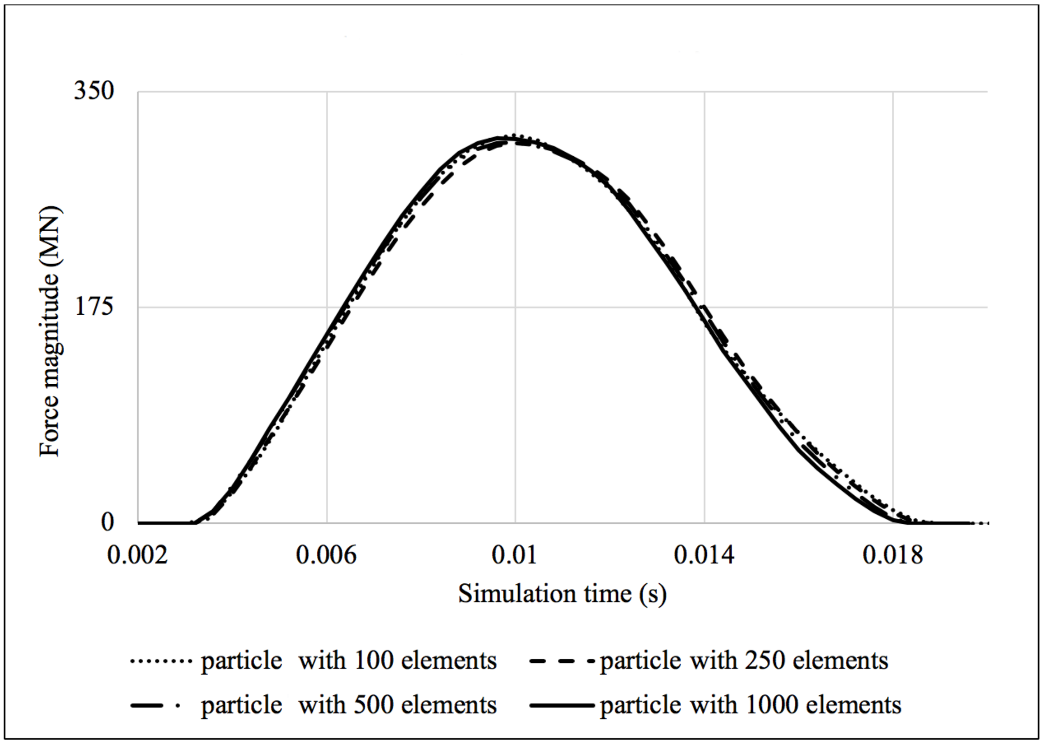

Figure 4: Overlapping impulses during a collision event

Although in some instances the collision repose is comparable between different mesh resolutions, for a number of particles, the response had dissimilarities. These can be attributed to the following:

The simplification process has changed the geometry by collapsing, altering or altogether removing asperities resulting in change of physical properties, such as dimensions or overall volume, of the particle. Consider the collision response shown in Figure 5, where the particle has undergone simplification such that the highest asperity, as measured from the average asperity height above the surface of a particle discretized into 100 elements, has undergone a reduction by 8 percent. This resulted in the alteration of volume of the particle by about 4 percent and a shift of its center of gravity by 4.5 percent. This can delay or accelerate the first contact collision depending on the discretization level, which is exhibited as a shift of the impulse curves. Note that the peak force varies no more than 5 percent across the various discretizations and the area under the curve remained within 6 percent across all impulse responses.

Another reason for the discrepancy in the impulse curves can be attributed to the contact mechanism that is used by the FEM/DEM system. The simplification process used to generate the particle surface may have changed the continuity property of the mesh. This resulted in fewer contacting nodes that can be detected by the algorithm for lower resolution models, while particles with higher resolution (more elements) provide more contacting node couples for the detection process. This difference is exhibited by a longer contact duration for particles with higher resolutions, which makes them more likely to have a deeper penetration into each other.

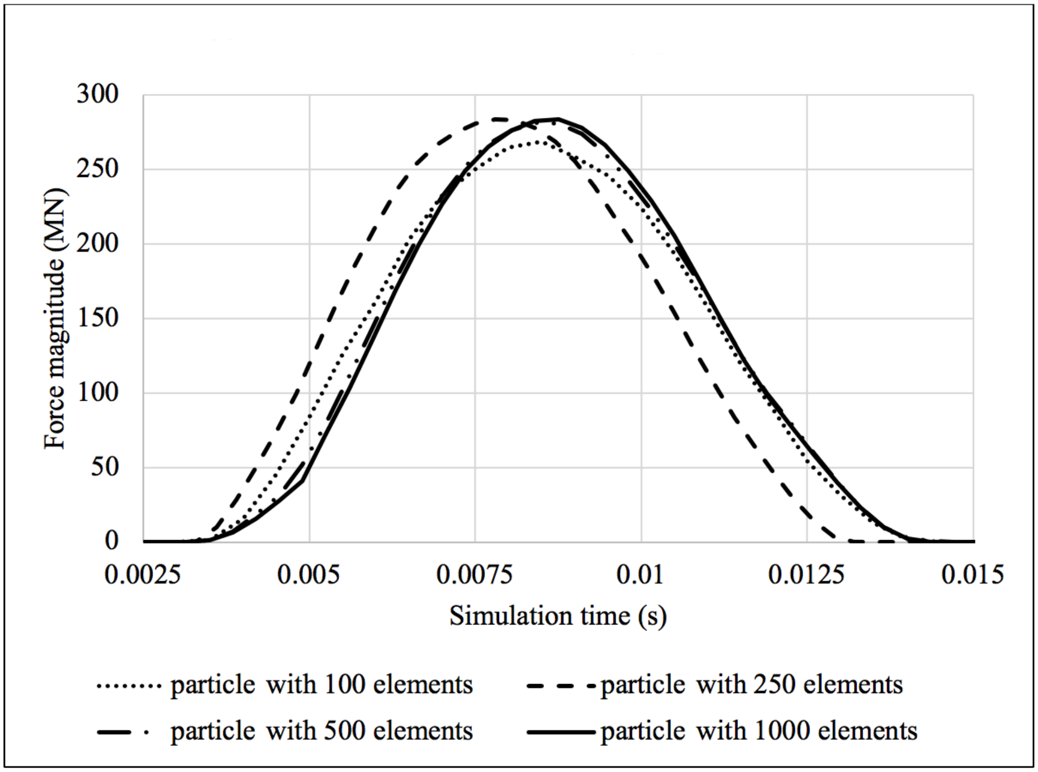

Figure 5: Shifted impulses during a collision event

The third reason for explaining differences is connected to the mesh simplification process that influences the position of a particle's center of gravity. Since the simplification process alters the geometry resulting in slight loss of gain of volume, the center of gravity varies from model to model. In the simulations, particles were placed at the same location as the center of gravity of the highest resolution particle was located. This choice, coupled with the reduction of asperities, resulted in earlier/later contact times and changes in contact durations. This was due to the algorithm that is used for calculating the total contact force exerted from target triangle onto the edge of contactor triangle, which is governed by the area of potential that is calculated by the interpolation between the edge's nodes and the central node corresponding to contacting triangles, as discussed in Equations 2-5.

As shown in Figure 6, some resultant force plots have a "tail", which means that the collision events are not the same as those have been discussed above; they are neither a simple "collide and detach" events, nor a "collide and re-contact with a small rotation" ones. The reason for these situations is due to the large deformation of the particle with different number of elements; particles have relatively larger contacting areas, as compared to other particle collision events, and relatively larger deformations were observed combined with a small rotation occurring during the collision event, but without separation of the particles. Thus, the collision process will be elongated comparing to those with sharp edge contact and quick detachment.

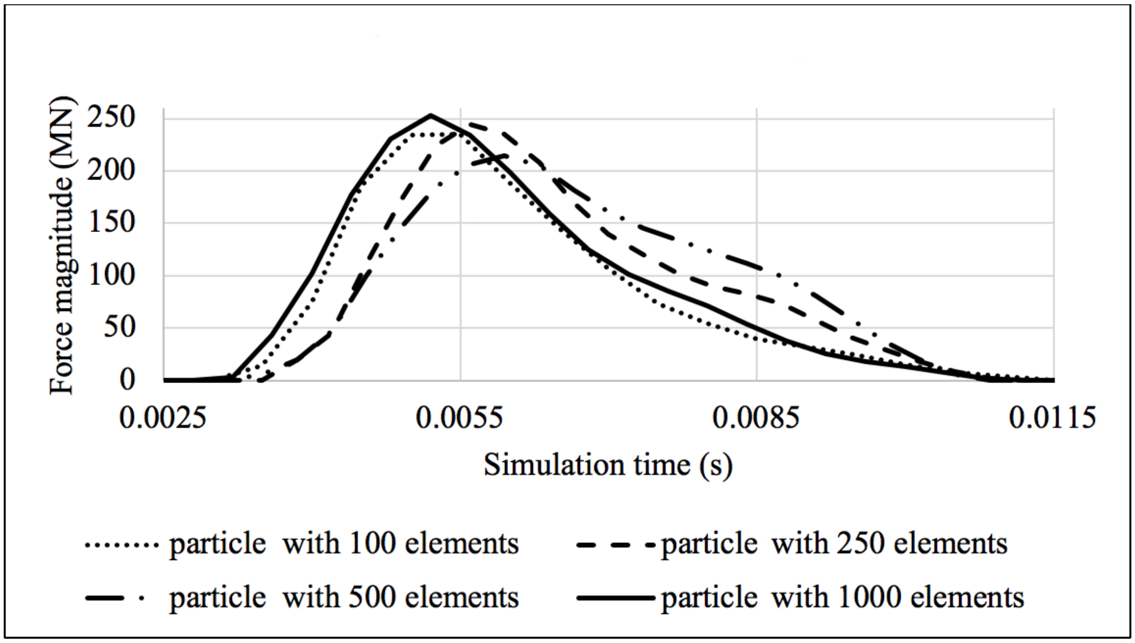

Figure 6: Impulses with “tails” during a collision event

Having assessed the collision response between a particle and a solid block and identified reasons for discrepancies between impulse curves, it can be concluded that increasing the element discretization often results in better resolution of the event with respect to contact forces. However, it has to be appreciated that finer discretizations could affect the solution time. Thus, for each simulation, the actual computation time spent by the CPU was recorded as well. Figure 7 summarizes the average simulation times across all 50 particles. For particles discretized into 100 surface elements, the average simulation time to resolve a collision was 4 seconds. However, when the discretization was increased to 250 elements, the CPU time increased almost by 8-fold. For discretizations with 500 elements, the solution time was very similar to the previous case. But when the discretization reached 1000 elements, the average solution time rose to 572 seconds, which is an almost 150-fold increase over the coarsest discretization with 100 elements. To interpret these numbers, one has to appreciate that the surface discretization (100, 250, 500 and 1000 triangles) leads to the generation of many interior tetrahedra and nodes. Although the increase in interior nodes does not affect the DEM simulation considerably since the interpenetration seldom goes deeper than one element, it has a considerable effect on the FEM computations since there are three degrees of freedom (x,y,z) for each additional interior node, leading to a potentially quadratic increase in solution time for the FEM.

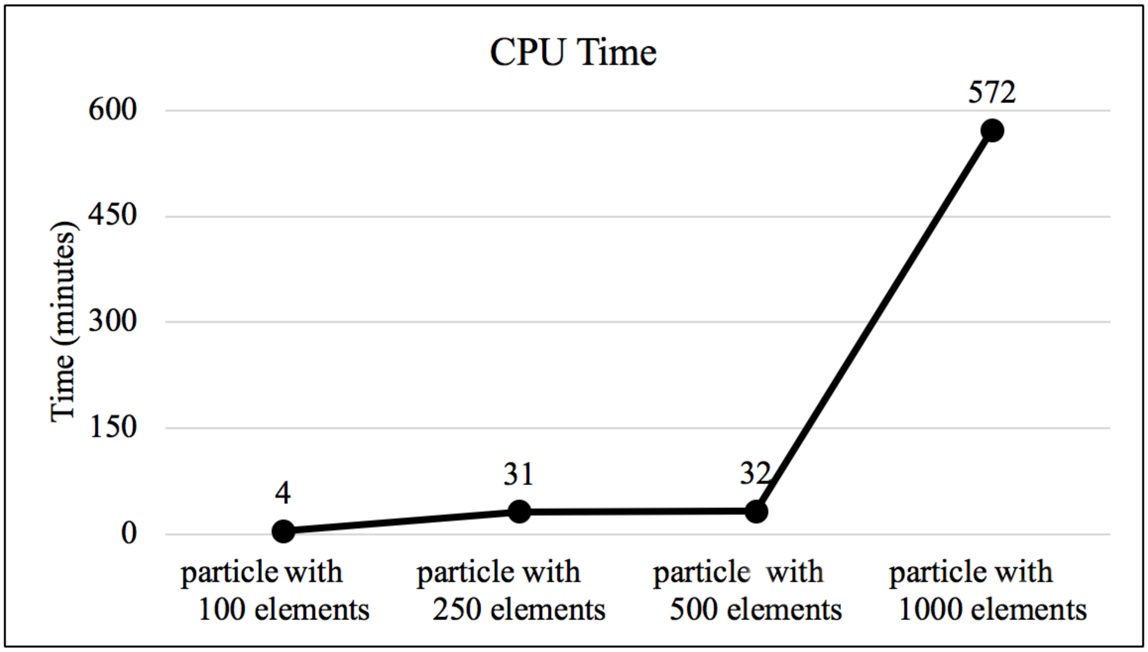

Figure 7: CPU runtimes for various discretizations

4 CONCLUSIONS

The mechanical behaviour of granular materials can be characterized by inter-particle collisions and the deformation of particles themselves in response to these events. As with many computer simulations, the more refined is the representation of a domain, be that a particle or a continuum, often a better approximation is obtained. However, this is achieved at a cost of increased computational resources and time. Considering the collision of granular particles, like railway ballast, the surface asperities play an important role in the force magnitude and distribution during an interaction. It is relatively hard to quantify the effect of surface detail; thus, this paper considered a set of particles, obtained via 3D scanning, and simplified their geometry for use in a combined DEM/FEM simulation. The results have revealed that the collision response can be dependent on the amount of surface detail and four categories of collision events were quantified. In addition, the effect of particle discretization on the computation time was investigated as well. It can be concluded, that beyond a certain point the added benefit of using a higher discretization is severely reduced due to the time it takes to run a simulation. Therefore, as a guideline, it is recommended to keep the particle discretizations within a range of few hundred surface triangles in order to preserve the quality of the simulation results, yet complete the simulation in a reasonable time.

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REFERENCES

Cundall, P. and Strack., O. 1979. A discrete numerical model for granular assemblies. *Geotechnique,* **29**(1), 47-65.

Hogue, C. 1998. Shape representation and contact detection for discrete element simulations of arbitrary geometries. *Engineering Computations,* **15**(10), 374–389.

Johnson, K. 1985. *Contact Mechanics*. Lundun: Press Syndicate of the University of Cambridge, UK.

Matuttis, H-G. and Chen, J. 2014. *Understanding the Discrete Element Method: Similation of Non-Spherical Particles for Granular and Multi-body Systems*, John Wiley & Sons, Singapore.

Munjiza, A., Owen, D.R.J., and Bicanic, N. 1995. A combined finite-discrete element method in transient dynamics of fracturing solids. *Engineering Computations*, **12**(1), 145-174.

Munjiza, A. 2004. *The Combined Finite-Discrete Element Method*, John Wiley & Sons, Ltd., London, UK.

NextEngine Inc. 2014. NextEngine 3D Laser Scanner. Retrieved from NextEngine 3D Laser Scanner Web site: http://www.nextengine.com/

O'Sullivan, C. 2011. *Particulate Discrete Element Modelling: A Geomechanics Perspective*, Spon Press, London and New York, USA.

Xiang, J., Munjiza., A. 2008. *Manual For The "Y3D" FEM/DEM Computer Program*. Queen Mary University of London (QMUL) & Imperial College of Science, Technology and Medicine (ICSTM), London, UK.