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Accurate modelling of particle shape effects in packed granular structures: a class of FEMDEM-suited particulate problems

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Abstract. In many granular applications, DEM capability is justifiably focusing on the dynamic solid particulate flow properties of systems in which millions of particles are involved and where the time of relevance is many seconds or even minutes of real time. Simplifying assumptions are made to achieve run completion in practical timescales. There are certain applications, typically in manufactured particles, where a representative pack is of the order of a thousand particles. More accurate capturing of the influence of complex shape is often necessary to model the topology of the void space e.g. for optimisation of fluid flow properties. Alternatively it may be the force or stress transmission through the contact points that is critical to avoid functional damage, or both structural stability and flow properties are the simulation purpose. The paper will draw out the importance of shape in the DEM community and narrow the scope to problems where shape is the key concern. It will then focus on the mono-size, mono-shape packing problem, highlight some of the key contributions and briefly illustrate FEMDEM applications where special shapes are needed for engineered granular packs.

Keywords: FEMDEM, particle packing, catalyst pellets, concave shape, non-spherical shape,

1 Introduction

In industry, the purpose of applying DEM is commonly to gain a better understanding of how to optimise a manufacturing process, one which invariably includes dynamic granular flows. To be representative, the simulated particle numbers involved are typically many (tens or hundreds of) millions and the granular

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flow process of interest for simulation may have a duration of many seconds or minutes, e.g. sieving/screening, hopper/shute/belt conveying, crushing, milling, mixing, coating, tableting etc. In such cases, even with massively parallelised computer hardware, accuracy of the particle geometry and hence particle to particle interaction often has to be forfeited. Indeed, sometimes the governing physics is highly complex especially for fine particles dominated by adhesive forces so that non-spherical particle geometry is considered only of second order importance. Approximate matching of emergent properties after lengthy application-driven calibration is justifiably a success. An example might be multiphase fluid-coupled particulate flows in fluidised beds with free surface (Sakai 2016). To achieve run completion in practical timescales demanded by the engineer, simplifying assumptions are made to represent the particle shape and shape distribution and also the size distribution of the granular medium to be modelled, and this is especially so when dealing with natural systems of grains.

The packing process and packed topology of granular systems has been a target application of DEM methods ever since they were invented by Cundall and Strack (1979). The packing of particles and their packed characteristics, (e.g. see German's 1989 treatise on the subject), as compared with granular flows in general, is a branch of granular problem that is more amenable to complex particle shape simulation. Improvement in computation power, parallel technologies and advanced e.g. contact algorithms in DEM and FEMDEM, have combined to make sufficient improvements that they are impacting on packing applications used in industry. The need and a means to address the important role of non-spherical shape in gravity-dominated i.e. coarser particulates behaviour, was highlighted a decade or so ago (Latham et al. 2002; Latham and Munjiza 2004). Where the effects of complex shapes are of critical importance to represent a process with sufficient accuracy, extra computational effort must be expended on capturing that highly resolved shape with smaller shape-defining elements. Industrial packing structures that form by a fast container-filling deposition process that bring coalescing moving particles rapidly in real time to a rest-state and which do not involve too many particles are ideal target problems because the associated smaller time steps required for the smaller elements and accurate contact dynamics can still be achieved within reasonable run times. All the more so where the pack of complex shape bodies is itself a mono-shape and mono-size system, e.g. in catalytic reactors, as discussed below. For catalytic packed beds, the motivation relates to the need for an accurate capture of the topology of the void space for optimisation of gas flows and to the potential fragility of the catalyst support grains/pellets. In the specialised case of coastal structures the pack is built with concrete armour units and the stability of a pack under an oscillatory forcing wave-structure interaction is the problem. Both structural stability and flow through the pack is often the target of fluid-solid coupled simulation aimed at improved system design.

In natural systems of packed rock fragment grains, e.g. for study of soil or rockfill behaviour, progress has been made with highly sorted and rounded sand deposits, e.g. flow modelling in a numerical process model of a sandstone's structure where the grain pack was created with different particle shapes using clustered sphere DEM (Garcia et al., 2009). The problem of assigning representativeness to the population of grains selected for the simulation domain i.e. size distributions and shape distributions, surface texture etc. for a specific geotechnical design application is still largely an outstanding one, especially for material containing angular grains. Even with an extensive shape library of numerically realistic rock fragment grain shapes (e.g. Latham et al 2008), it is not trivial to determine the proportions and sizes of each numerical grain based on objective criteria geared to the delivery of an expected accuracy. This is a topic that requires further research. Rather than using DEM sedimentation process models to create soil and rock fabrics to investigate the effect of grain shape on strength and flow properties, direct sampling of the grain fabric from rock cores e.g. by X-ray CT scanning is an option, e.g. Taylor et al. 2015 captures a poorly consolidated sand fabric while Jia and Garboczi (2016) discuss shape acquisition and representation of realistic angular rock grains. However, the next step of translating the geometry into a computational mesh domain for further DEM type loading or CFD flow simulations is also not trivial. The paper continues with a short summary of available numerical methods for modelling packing processes before illustrating two applications requiring high accuracy in the complex shape representation.

2 Modelling methodologies for the effect of shape on packing

Packing algorithms for non-spherical particles that have superseded the popular type of frozen-once-placed ballistic deposition algorithm once appropriate for spheres (Aparicio and Cocks 1995) or sphere composites, can be divided as follows:

- Purely geometric types include random space filling and collective rearrangement, for example the ACS algorithm of Torquato and Jiao (2008) used to obtain densest random packings of Platonic and Archimedian solids. Voxel based methods (Jia and Williams 2001); these began as entirely geometric with the attraction of capturing any shape. Realism of such approaches has improved with the addition of some DEM-like interaction features to create DigiDEM however, contact force models are more limited than for sphere contacts (Caulkin et al., 2015).
- DEM based on extensions from the original spherical-based approach with geometrically determinate radial contact normals, e.g ellipsoids and superquadrics (Williams and Pentland 1992) as widely exploited in DEM technologies of Cleary's CSIRO group, and termed superellipsoids, e.g. Delaney et al., (2015), see also the review by Lu et al. (2012).
- DEM based on clustered overlapping variable size spheres (clumped spheres) Favier et al., (2001), Garcia et al (2009). These methods are the back-bone of commercial simulators such as PFC3D (by Itasca), and EDEM (by DEM Solutions) and can seem very impressive in

visualizations of conveying and packing simulations where realistic object outlines from CAD e.g. fastening brackets, or shape library particles with faces and facets are ‘draped over’ clustered spheres to hide the bumpy surface sliding mechanics being simulated. DEM for ‘spherosimplices’ such as spherocylinders or spheroplates e.g. formed by moving a sphere along a line or perimeter can approximate certain shapes.

- Polyhedral DEM where contact forces can be calculated between arbitrary shaped convex and concave polyhedra with overlapping volume or common plane area repulsive force formulations. Simple and fast solutions and linear scaling have been reported e.g. Smeets et al (2015). See also the contact force method of Elias (2014) who uses Voronoi tessellation methods to generate polyhedral shapes for ballast and rockfill applications.
- Combined FEMDEM approaches either (i) where to create arbitrary complex and convex particles, shapes are constructed from combinations of primitive concave polyhedra that can be rigid or deformable, e.g. 3DEC^{TM} (by Itasca), or (ii) by FEMDEM using a distributed potential contact force algorithm using surface triangular and volumetric tetrahedral meshes at the appropriate resolution to approximate the shape effects and where both deformable or rigid approximations may be suited depending on the application. Similar approaches have sometimes been referred to as multi-particle FEM (MPFEM) especially in the field of powder metallurgy where the focus is on plastic particulate properties (Gunner et al 2015).

For many applications with natural rock fragment shapes, the problem has been to introduce facetted angular particles and to solve the contact mechanics problem. Polyhedral DEM solvers handle better the angular contact interaction. To represent an angular source material in polyhedral DEM, the BLOKS3D DEM program (Huang and Tutumluer 2014) creates typically ten or so different digital simple facetted particles by iteratively slicing separate grains until optimally matching predefined descriptors of angularity, flatness and elongation of each of ten real aggregate particles, from which a representative digital sample is made.

A challenge for the FEMDEM methods, especially transient dynamic deformable simulations that track the stress waves inside the grains, is that the methods are relatively more expensive in terms of computational time, which limits the number of particles that can be considered or process time that can be modelled. Where the particles are known to have both smoothly curved and flat faces while also having sharp edges, such as cylinders, the number of tetrahedral elements to represent this particle geometry accurately may seem prohibitive. In this work, illustrative results of the parallelized FEMDEM code *Solidity* (see Xiang et al., this conference) developed at AMCG Imperial College are presented for two applications where close replication of geometry and resultant packed properties are essential.

3 Applications of FEMDEM using *Solidity*

Two very different applications featured in this paper are special cases where the system of interest can be meaningfully modelled with particles numbering some several hundred or a few thousand and the individual solid particle geometries themselves can be discretized using about 10^2-10^4 tetrahedral elements per particle.

3.1 Pellets for Catalytic Reactors

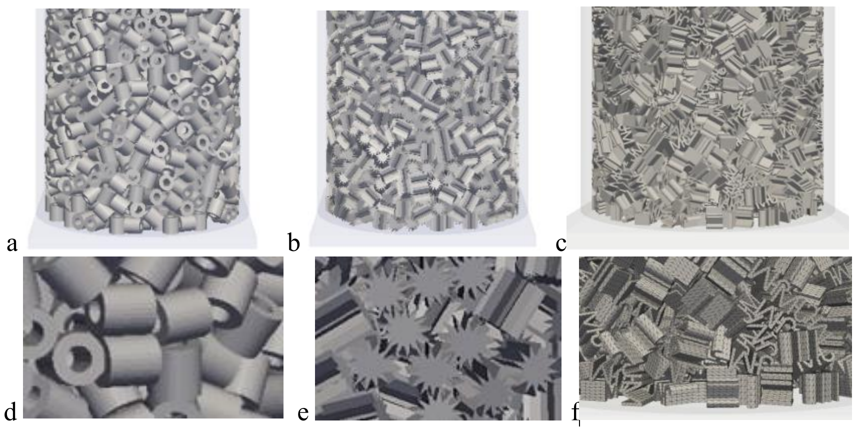

Fig. 1 Packing structure at bottom of a cylindrical container simulated for the three particle geometries; a) one-hole cylinders, b) gear-cog shaped pellets c) lettering pellets made from CAD file extrusion; d) e) and f) as above showing close ups with tetrahedral mesh elements.

Packed bed pellets, sometimes referred to as catalyst supports, will typically be made from porous ceramic materials to enhance reactions of the catalyst. They will be shaped to offer a high surface area, to enhance reaction rates as pressurized fluids flow up and through a high temperature packed bed. However, the bed must have the correct permeability and not unduly retard the high temperature gas flows. Breakage of pellets into fragments causes reduced flow efficiency, uneven flow and excessively hot spots can result which in turn can adversely affect the steel container walls. Stresses additional to those from self-weight can build up from thermal stresses and especially by shrinkage of the steel cylinder itself if the catalyst process is shut down and reverts to ambient temperatures. To better understand the role of pellet shapes and the strength and physical properties of the support medium on the intricate coupled behavior, modelling the thermal conduction and fracture behavior of the pellet pack would be a distinct advantage, ideally also coupled to the turbulent fluid flows. Models for heat flow within pellets with arbitrary surface boundary conditions and across multi-body contacts have been developed for FEMDEM *Solidity*, (see Fig. 2 and Joulin et al., 2016 this conference). FEMDEM models will therefore in principle be able to simulate thermal stresses related to volumetric strains within the pellets that can be automatically combined with stresses generated by the contact force network. Fig. 3 shows stress chains resulting from a gentle compression of packed cylinders. For a simpler 2D illustration of the role of stress chains in FEMDEM simulations, see Guises et al., 2008.

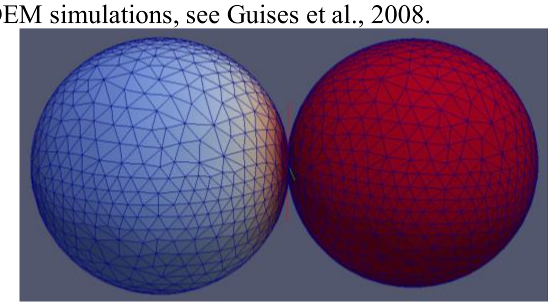

Fig. 2 Heat conduction from hot sphere on right contacting sphere on left, model implemented in FEMDEM Solidity, see Joulin et al. 2016 this conference, paper yyy.

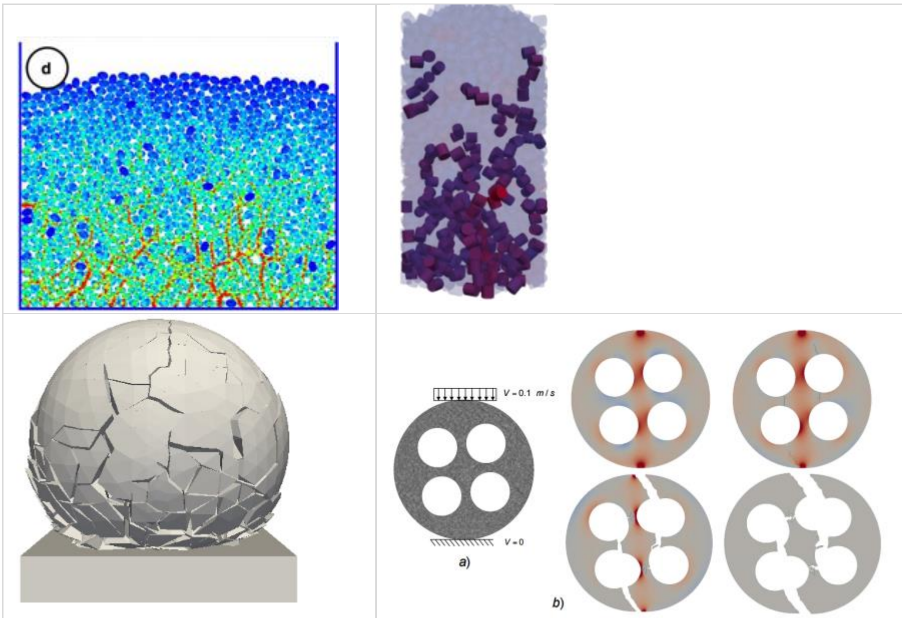

Fig 3. Analysis of stress and fracture in particles with FEMDEM. top left: Stress chains in elliptical packed beds captured by FEMDEM in 2D: Guises et al, (2009); (top right) 3D. Bottom left: 3D fracture model, Guo et al 2015; Bottom right disc with holes that improve surface area but make pellets more prone to fracture, Farsi et al 2015.

A further advantage of FEMDEM is the potential to apply different constitutive models for the deformation response to stresses. *Solidity* supports validated 2D and 3D fracture models (Farsi et al. 2015, Guo et al., 2015a,b) applicable to granular breakage and fragmentation in multi-body loading. For simulations that capture internal particle deformation and stresses, computational demand is about an order of magnitude greater than with rigid particle approximations. However, importing packed geometry meshes created using rigid modelling for loading in a fully deformable FEMDEM model is an efficient work flow to examine stresses within larger realistic pack systems. Alternatively, if the particle materials are elastic-plastic, a range of plasticity models have been implemented in FEMDEM (Karantzoulis et al 2013) to predict ductile multi-body compaction or extrusion. The large strain plasticity capability in *Solidity* is also applicable to catalyst pelletization (and other powder compaction processes) as pellets are formed from compacted soft aggregates.

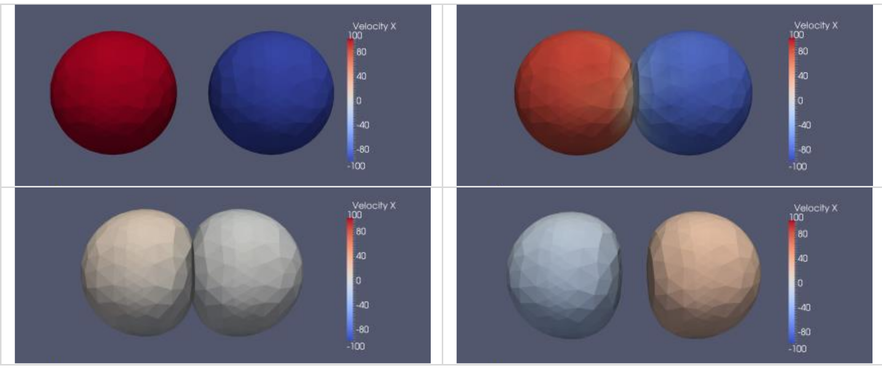

Fig.4 High speed collision of two plastic spherical bodies (Karantzoulis et al., 2013), illustrating plastic model capability of FEMDEM Solidity for modelling powder compaction in tablet and pellet forming.

3.2 Concrete Armour Units

Harbour breakwaters are often constructed with concrete armour unit layers. When designed appropriately these gigantic granular systems can withstand the wave forces for a predicted sea state or design storm. Breakwater armour system design is largely empirical and would be transformed by a better fundamental understanding of loads and restraining forces. Numerical models based on FEMDEM are leading the solids modelling effort as they can handle the complex shapes and contact forces most realistically. The units are very massive (10 to 100 tonnes) and are cast with unreinforced concrete. The units available have widely varying shapes, are if left loose and poorly interlocked they may be dislodged, or simply rock and are potentially fragile. They are placed with irregular orientations

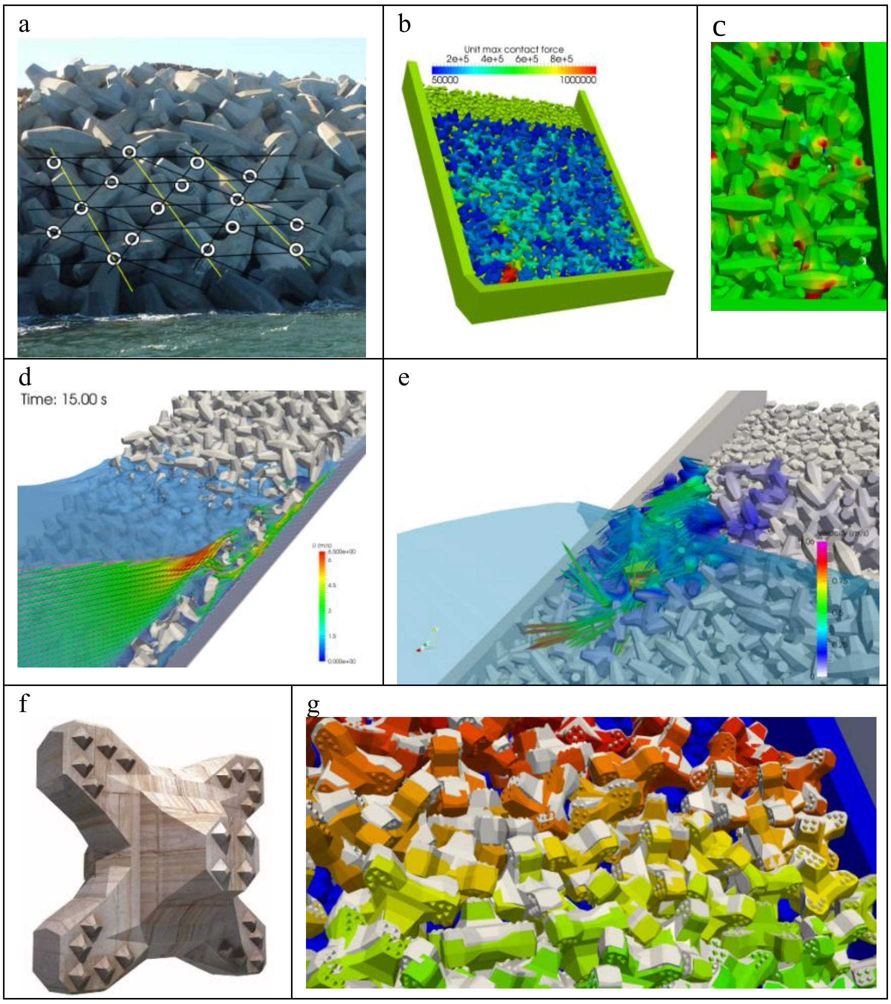

Fig. 5 Application of FEMDEM to breakwater stability prediction. a) breakwater with Core-Loc units in row-column pattern b) model of breakwater section ~ 10^6 elements with statistics of maximum contact force c) tensile stress details; d) pressure and velocity time history for wave-structure interaction sequence modelled with IHFOAM, e) movement of armour units modelled with FEMDEM *Solidity* wave proxy f) Accropode II^{TM} unit g) position of armour units before (white) and after (colours) storm wave sequence.

by crane in rows and columns to a GPS system grid to yield a specified packing density. Numerical models allow statistical parameters such as coordination number, contact forces and tensile stresses of the static pack to be analysed (Latham et al, 2013) (Fig. 5a, b, c). Random wave sea states have been modelled to interact with the FEMDEM breakwater topologies by applying the wave simulation code IHFOAM (Higuera et al 2013) to obtain the time history of velocities and pressures of the turbulent flows. After calibration the forcing hydraulic lift and drag forces are obtained. The hydraulic forces are summed together with the solids forces governing motion in the FEMDEM code *Solidity* in an application termed the wave proxy which has been used to predict stability and armour unit movements, for different armour pack characteristics, for one hour of a 100 year return period storm, (Latham et al., 2015) (Fig. 5d and e). Innovative shapes of units are frequently proposed. To encourage their take up by designers and clients when there is no record of site performance, demonstration by scientific principles embodied in mechanical simulations and analysis tools may prove more effective than empirical model testing where scale effects may not be accounted for. For example, the design of units with specially added geometric features such as the sacrificial friction studs of Accropode II^{TM} can be interrogated by advanced modelling (Fig. 5 f, g).

4 Discussion and Concluding Remarks

To illustrate how simple it is to explore ideas of science and engineering with FEMDEM *Solidity*, two armour unit types were modelled as catalyst pellet-size particles of equal volume and deposited from an identical evenly spaced array into a cylinder to compare random packing behavior for two armour unit shapes used widely in coastal structures, Core-Loc and X-bloc (Bakker et al 2004). When deposited in bulk with random deposition, the packing density and topology appear quite different for each unit, for identical friction coefficients; clearly there are fundamentally different packing phenomena affecting the packing characteristics for each unit (Fig. 6) but the collision dynamics involve only very small masses. Many scaling issues are of potential interest: at full-scale, the dynamic stresses would render the whole as a pile of concrete fragments, if sufficient computer resources could track the 3D fracture modelled response. When full-scale units are placed gently one by one in breakwaters using regular grid spacing and semi-random orientations, single layers made of both types of units and similar packing densities are found to perform with very similar stability under wave action. This suggests that the placing by the crane operator has over-riding importance and the highly non-random nature of the rotations, slinging conventions and final positioning are critical for these units to work and interlock effectively. The bulk packing simulation result such as those in Fig. 6 together with a whole suite of analysis tools to interrogate them may be just the start of a new journey of enquiry. If nothing else, they have the hallmarks of an excellent FEMDEM validation study.

In summing up, it is proposed that we can now identify a distinct (FEMDEM-suited) class of complex shape particulate problems with two properties: firstly, a high accuracy in shape representation and contact mechanics is essential to the simulation user and secondly, the number of particles are relatively few such that industrially useful simulation results are achievable in practical runtimes on affordable hardware – i.e. a company can improve the profitability of its industry/organization by adopting such simulation tools. DEM has made its mark in industry already but not in this utility class of particulate problems. The applications illustrated here are catalyst packing behaviour and armour unit pack stability and the most suitable software, we argue, will be of the FEMDEM type. For both these illustrated problems, packing characteristics can be indicators of structural stability and/or resistance to flows through the packs which can be readily investigated with sensitivity analyses. Computational power of affordable multi-core desktops are today sufficient for FEMDEM codes (with parallelized architecture and advanced interaction and search algorithms together with algorithmic efficiencies) to tackle industrial problems with computer runs of about 1 day or less for a certain class of problem. These problems are the rapid packing of relatively few particles of complex shape that can be captured within the computational domain with ~10^5-10^6 tetrahedral elements. It is suggested that several industrial packing problems are now in this utility class already, or will be in the very near future, together with the two problems highlighted in this paper.

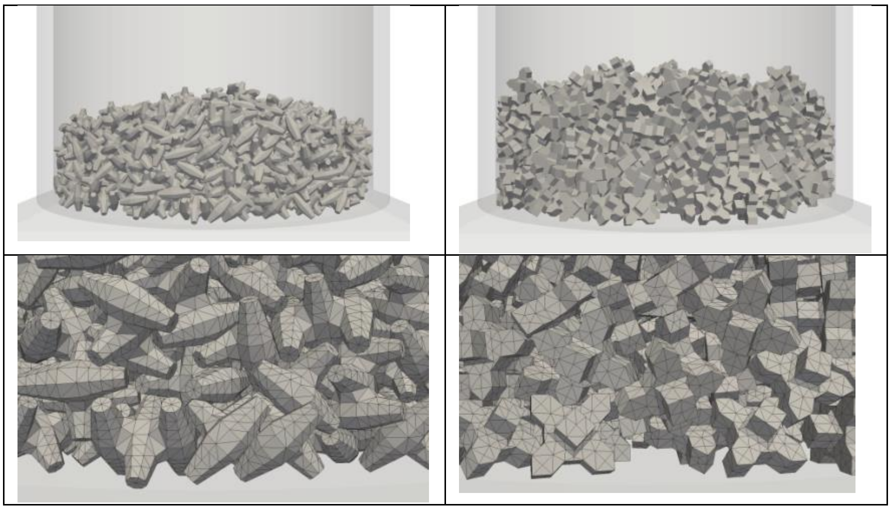

Fig. 6 FEMDEM simulation showing packing structure of concave particle geometries, Core-Loc™ left and X-bloc® right, widely used for single layer armouring of breakwaters. Even deposition of random orientation particles of ~ 3mm width, i.e. ~1000 times smaller than typical breakwater prototype sizes.

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