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OPTIMAL PACKING OF POLY-DISPERSE SPHERES IN 3D: EFFECT OF THE GRAIN SIZE SPAN AND SHAPE

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Abstract. In this work, we explore the effect of the grain size distribution (gsd) on the packing of 3D granular materials composed of spheres, and find the optimal packing with the highest density as a function of the gsd parameters.

1 INTRODUCTION

Granular media are materials composed of interacting bodies with many types of possible microscopic parameters that impact the global response of the system under given external conditions. In particular, poly-dispersity, which characterizes the differences in size for the constituent grains and can be described by the grain size distribution (gsd), has been shown to strongly influence the packing properties of the system.

In this work, the gsd is modeled as a truncated power law that can be characterized by its shape (exponent, η) and its size span (ratio of the larger to the smaller particle size, λ), and is defined as

$$\rho = \left(\frac{d - d_{\min}}{d_{\max} - d_{\min}}\right)^{\eta} = \left(\frac{\frac{d}{d_{\min}} - 1}{\lambda - 1}\right)^{\eta}, \tag{1}$$

where $d_{\min}$ ($d_{\max}$) is the minimum (maximum) diameter in the sample, and ρ is the fraction of volume occupied by particles of diameter d. This distribution arises as a result of the previous works of Fuller, Thompson, and Talbot [1, 2, 3] (experimental) and those by Furnas [4, 5] (theoretical) between 1907 and 1931.

One common and important question is if there is an optimal gsd that generates the best packing measured in terms of some packing variables such us the packing fraction (or density), the local connectivity [6, 7] and anisotropy [8, 9, 10], the force distributions and so on. For instance, Fuller and Thomson found [1], more than a century ago, than an optimal packing with the densest state could be obtained with an exponent of $\eta \simeq 0.5$. This has been verified [11, 12] in 2D simulations comprising systems with large size spans, up to $\lambda = 32$.

Large size spans in three dimensions are hard to simulate due, in part, to the large computational resources involved. Previous work had focused in 2D [13, 14] ($\lambda \simeq 8$), [15] ($\lambda = 3$), and with special mention to the works of Voivret where really large size spans where explored for discs ($\lambda \simeq 20$) [16, 17] and polygonal particles [18, 19], and recent works with larger λ [11, 12, 20] and in 3D [21].

In this work we explore very large three-dimensional samples composed of frictionless spheres under isotropic compression and with different gsd. The shape of the distribution was in the range $\eta \in [0.1, 0.2, \dots, 0.9, 1.0]$, while the size span was changed as $\lambda \in [2, 4, 8, 12, 16, 24, 32]$. These values include common distributions and explore some regions not commonly simulated. For instance, $\eta = 1.0$ corresponds to a uniform by volume distribution. For large λ and small η, the systems were composed of up to 400000 particles to represent the gsd accurately (maximum difference less than 5%). Some of those systems, when compressed, also generated more than one million contacts. Simulations were performed using the LIGGGHTS [22] package on a multicore server. Figure 1 shows snapshots of the 3D systems for fixed $\eta = 0.5$ and $\lambda = [4, 32]$. Only the particles away from the walls by $1.5\langle d \rangle$ were used for processing.

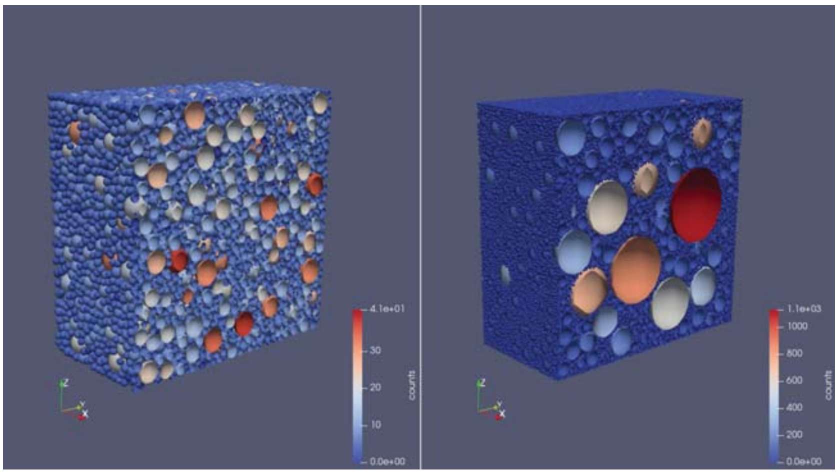

Figure 1: Screenshot for $\eta = 0.5$, and (left) $\lambda = 4$ and (right) $\lambda = 32$. The systems were cut in half to show the inner particles. Color represents the number of contacts. For the $\lambda = 32$ system, the larger particles could have more than 1000 contacts.

We found that values around $\eta = 0.5$ produce packings with the highest densities, which is in agreement with the century-old Fuller-Thomson distribution. Also, the proportion of floating particles could reach values as high as 90% for large λ, while the mean coordination number decreases drastically. These results allows, for instance, to design packings which could be better densified and connected just by controlling its generating gsd. Finally, the very high number of floating particles, or, equivalently, the very low mean coordination number, means that some systems could fracture under some mechanical conditions since the forces will be focused on a small number of particles.

The paper is structured as follows: in section 2, we describe the numerical method and the sample setup. In section 3, we show the main results for the density and the local ordering as functions of the gsd. Finally, in section 4, we present some conclusions and suggestions for future work.

2 Numerical method

Simulations were carried out by using the soft-particle discrete element method. Here the particles are modeled as bodies that deform a little (given the Young modulus) when touching each other, and the repulsion force is proportional to a power of that deformation. In particular, we used the so called Hertz model [22, 23, 24, 25]. The particles were spherical, without friction, and compressed isotropically on a cubic domain.

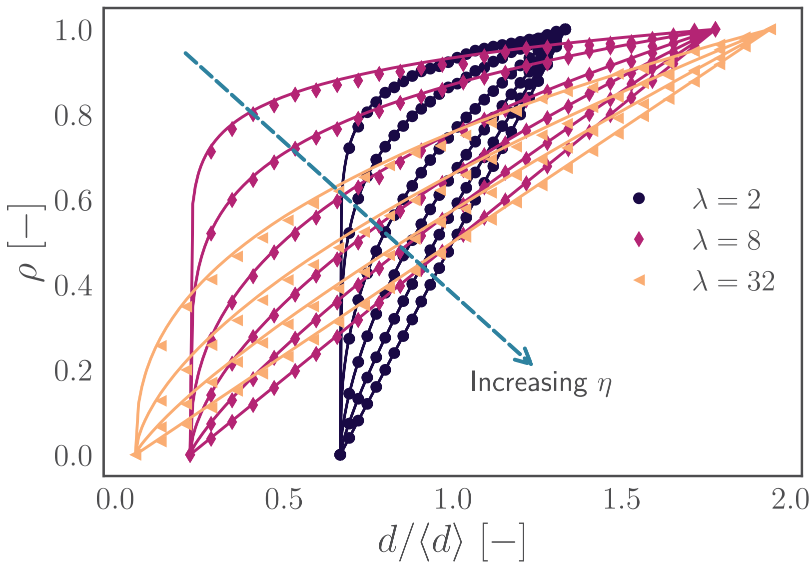

Figure 2: Grain size distribution (1) for some values of λ and all η. In all cases, the average diameter $\langle d\rangle = 0.5(d_{\min} + d_{\max})$ was fixed to the same value.

We randomly generated radius according to the gsd (1) and accepted configurations only when the maximum difference between the numerical and the theoretical gsd was smaller than 5%. The generated sample was equilibrated inside a cubic box and then compressed isotropically, slowly, until reaching mechanical equilibrium. The simulation was stopped when the cundal parameter, defined as the sum of the net force per particle over the sum of the net force per contact was smaller than 0.001, which indicated mechanical equilibrium. Data processed to extract the results shown below was filtered to be one mean diameter away from the walls and, when needed, excluding the floating particles, defined as particles with only 0 or 1 contact.

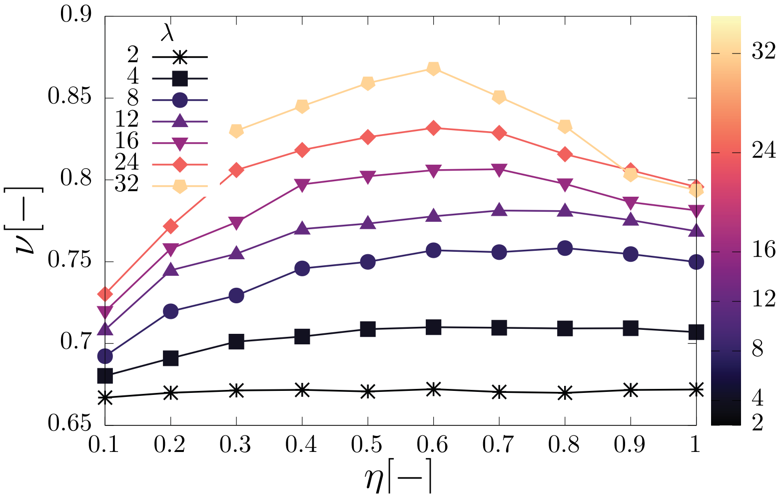

Figure 3: Packing fraction ν for several λ and η, after an isotropic compression.

3 Density and connectivity

Figure 3 shows the packing fraction ν (volume of particles over volume of the packing)

$$\nu = \frac{V_p}{V}, \tag{2}$$

as a function of both λ and η. We can see that for all λ, there is always and optimal $\eta \simeq 0.5$ where the packing fraction is the largest, and this is more notorious for larger λ. This result agrees with the Fuller and Thomson finding, giving it support now for 3D. This shows that, to maximize the density it is not enough to have a large λ, but also and intermediate value of η. Allowing to increase the proportion of small particles helps filling the voids left but the larger particles, but when η is too large then the space filling is not optimal again.

One measure of the connectivity of the system corresponds to the proportion of floating particles, or, equivalently, the mean coordination number, which is the mean number of contacts per particle. Both of them give a first order idea on how well connected is the system to distribute the external forces among the particles.

The proportion of floating particles, κ, is defined as

$$\kappa = \frac{N_f}{N_p}, \tag{3}$$

where N_f is the number of floating particles and N_p is the total number of particles. A particle is defined as a floating particle if its number of contacts is 0 or 1, so it cannot be a part of a force bearing chain inside the sample.

Figure 4 shows the percentage of floating particles as a function of both λ and η. This proportion can reach values of up to 90%, which in turns decreases the mean coordination number to values around 0.5, when all particles are included in the computation. In fact, when the floating particles are excluded, the mean coordination fluctuates around 6,

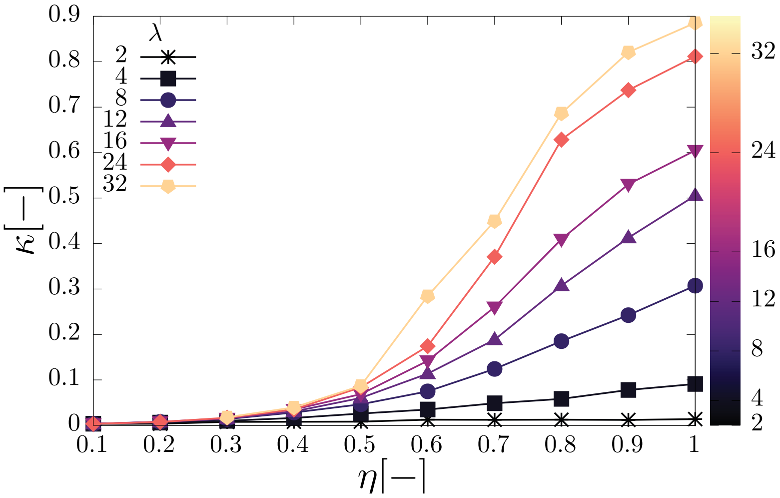

Figure 4: Proportion of floating particles, κ, for several λ and η, after an isotropic compression.

as expected for the isostatic condition. This high percentage of floating particles looks surprising, and has some mechanical implications. For instance, it implies that the forces inside the packing are distributed among a small subset of the particles. This makes this kind of systems more likely to fracture.

4 Summary and conclusions

We have studied three-dimensional frictionless systems with very large polydispersities characterized by the grain size distribution (1) with shape $\eta = [0.1, 0.2, \ldots, 1.0]$, and size span $\lambda = [2, 4, 8, 12, 16, 24, 32]$. The systems were compressed isotropically until mechanical equilibrium was reached.

We found an optimal packing where the density is maximum and correspond to eta = 0.5, which is Fuller and Thomson.

The density of the system, measured by the packing fraction ν, depends strongly on λ and η. In particular, we found that for almost all system, specially large λ, there is always an optimal packing with the largest density around $\eta \simeq 0.5 - 0.6$, which is close to the Fuller-Thomson distribution and confirms that this shape parameters generates the densest packing.

Furthermore, after these optimal η values, the proportion of floating particles κ increases strongly, reaching values of up to 90%. This implies that $\eta \simeq 0.5 - 0.6$ corresponds not only to the densest packing but also marks the transition from a well connected packing to a packing where a small subset of particles participate on the force bearing networks. The high percentage of floating particles make the systems more fragile since they might be more likely to fracture the grains.

The present results support the design of granular packings from the actual gsd, choosing λ and η to reach a target density and connectivity. This can be extended to systems with friction, or with different mechanical solicitations, like simple shear or triaxial tests.

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