# Optimal packing of poly-disperse spheres in 3D: effect of the grain size span and shape

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## ABSTRACT

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 a truncated power law that can be characterized by its shape (exponent, $\eta$) and its size span (ratio of the larger to the smaller particle size, $\lambda$), and one common 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, 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 [2] in 2D simulations comprising systems with large size spans up to $\lambda = 32$ .

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 $\eta \in \{0.1, 0.2, ..., 0.9, 1.0\}$, while the size span was changed as $\lambda \in \{2, 4, 8, 12, 16, 32\}$. For large $\lambda$ and small $\eta$, the systems were composed of up to 400000 particles to represent the gsd accurately. Those systems, when compressed, also generated up to one million contacts. Simulations were performed using the LIGGGHTS package on a multicore computer.

We found that even in three dimensions there is an optimal gsd, with shape parameter $\eta = 0.5 \sim 0.6$ as the Fuller-Thomson distribution. Also the proportion of floating particles could reach values as high as 90% for large $\lambda$, while the mean coordination number decreases drastically. Furthermore, the radial correlation function showed that local ordering was easily erased just by increasing a little the size span $\lambda$. These results allows, for instance, to design packings which could be better densified and connected just by controlling its generating gsd. Also, the extension to three dimensions with large poly-dispersities support the original results from Fuller-Thomson. 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.

## REFERENCES

[1] Fuller, W. B., & Thompson, S. E. (1907). The laws of proportioning concrete. Transactions of the American Society of Civil Engineers, 59(2), 67143.

[2] Estrada, N., & Oquendo, W. F. (2017). *Microstructure as a function of the grain size distribution for packings of frictionless disks: Effects of the size span and the shape of the distribution.* Phys. Rev. E, 96(4), 042907. https://doi.org/10.1103/physreve.96.042907