Multi-Sized Sphere Packing

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Abstract

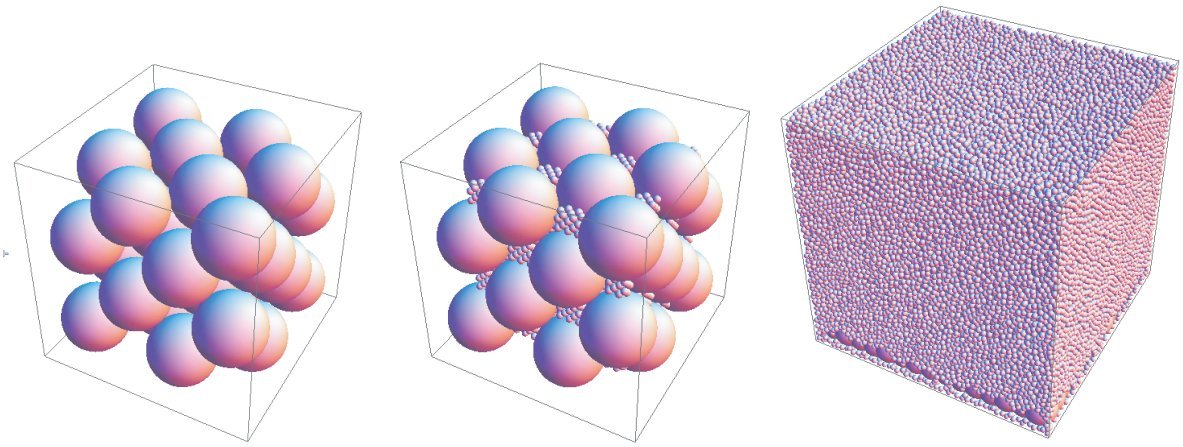
It is known that dried concrete contains numerous pores which allow for concrete deterioration by providing chloride ions a path to the supporting rebar. A new method called electrokinetic packing using nanoparticles to fill the pores was proposed and at least two different sizes of nanoparticles must be used.

We found a simple approximate relation for the two sizes of spheres that provide a high density in the multi-sized random sphere packing problem into a container C by using only the parameter $\beta = B/V$ where B is the surface area of C and V is the volume of C.

1 Regular Crystal Structures and Random Packings

A highest density for mono-sized sphere packing in R^3 has been considered for centuries. Kepler's Conjecture (1611), proved by Hales (1998): The highest packing density of spheres in the 3-dim space is $\frac{\pi}{\sqrt{18}} \doteq 0.74048$. For example, the Face-Centered Cubic Crystal Structure in the Figure provides this density. If we add smaller spheres to pack the vacancy of the previous packing, we can increase the density further. If we pack infinitesimally small spheres into the previous structure, then we can reach to the limit density $1 - \left(1 - \frac{\pi}{\sqrt{18}}\right)^2 \doteq 0.93265$

In application, nanoparticles are randomly packed and the density will be lower than the highest density 0.74048 of regular packing. In literature, there are two distinct random packings when we pack objects in a container: Random Close Packing(RCP) and Random Loose Packing(RLP). In RCP, a higher packing density is obtained by shaking the container after a random packing than RLP where no shaking of container is performed. In 1969, the approximate density 0.64 of RCP of mono-sized spheres was obtained from the experiment packing steel spheres to a container and shaking the container.



We will now describe our packing methods and results. Our method uses a deterministic algorithm with a random initial case. As a result we can achieve varied results using multiple initial conditions. We first determine all the positions where a new sphere touches 3 old spheres which we refer to as pits.

We place the center of a new sphere at the pit whose z-coordinate is the lowest among all possible pits.

For example, we pack spheres of radius 0.02 to a $2 \times 2 \times 2$ cubic container C having a random shaped base (figure in the previous page). The following figure(left) shows the packing density as a function of the distance from the boundary of C. The average of the packing densities about the center of C is 0.604. By assuming the average density to be 0.604, shown by the large lightly(blue) shaded region, we can calculate how much we should consider as a loss around the boundary of C. As a result of our estimate, 0% to 30% of the radius from ∂ C can be subtracted, shown as the smaller darkly(red) shaded region. We did this experiment for several different shapes and sizes of C and obtained almost the same results as above.

From now on, let V be the volume of a container C and B the surface area of C. Suppose we pack a container C with identical spheres of radius r. From the experiment, we can approximate the influence of the ∂C as a loss of $0.3r$ neighborhood (See the previous graph) or $0.3Br$ volume reduction and use the average density 0.604. More precisely, we can assume we pack spheres in a space of having the volume $V - 0.3Br$, instead of V, with the average density of 0.604. Therefore, the total density after random loose packing of spheres with radius r can be approximated by $\frac{0.604(V-0.3Br)}{V} = 0.604 - 0.1812\beta r$. where $\beta = \frac{B}{V}$.

We pack a container C with spheres of two different sizes with radii $r_1 > r_2$. First, we pack C with large spheres having radius r_1. The total volume of large spheres: $(0.604 - 0.1812\beta r_1)V$ The total surface area of large spheres is $(0.604 - 0.1812\beta r_1)V\frac{3}{r_1}$. The volume remaining is $V_1 = V - (0.604 - 0.1812\beta r_1)V$ and the new surface area which now includes the packed sphere surfaces is now $B_1 = B + 3(0.604 - 0.1812\beta r_1)V/r_1$. Now if we pack small spheres of radius r_2 into C_1, then the total volume is $0.604(V_1 - 0.3B_1 r_2)$. The total density after randomly packing spheres of radii $r_1 > r_2$ is

$$0.843184 - 0.0717552\beta r_1 - 0.0826997\beta r_2 - 0.328334\frac{r_2}{r_1}. \tag{1}$$

From this formula, we can see that the total density is maximized when $r_1 = 2.14\sqrt{\frac{r_2}{\beta}}$.

2 Computational Experiments

We assume that the small size of radius r_2 is fixed at 0.02. Then, the problem is to choose a radius r_1 to achieve maximal density when packing pores. In order to determine the optimal value, we run multiple simulations packing spheres in a rectangular box with a 2×2 base and determine the optimal values empirically. We limit the range of r_1 from 0.05 to 0.5. See the following figure (center). The solid curve shows the above approximation (1). The last figure is the packing of case $r_1 = 0.214$, which maximizes the value of (1).