Maximal Sphere Packing

Alec Jacobson, alecjacobson@nyu.edu

August 9, 2010

1 Packing a volume

Our goal is to pack a given volume, $V$, with uniform-radius (same-size) spheres. There are two flavors to this problem. (1) For a given volume, $V$, and a given number of spheres, $n$, what is the largest radii, $r$, those spheres may have and still all fit in the volume? (2) For a given volume, $V$, and a given radius, $r$, what is that largest number of spheres, $n$, that will fit in the volume. These two problems are essentially the same, but we’ll see where they differ a little in the result. If we accept the Kepler conjecture, then any packing of $n$ uniform spheres could at best give us a packing ratio of volume covered by spheres, $nS$, to the total volume, $V$:

$$\frac{nS}{V} = \rho_{\text{max}} = \frac{\pi}{3\sqrt{2}} \approx 0.74$$

where $S$ is the volume of sphere with radius $r$, that is:

$$\frac{4}{3}\pi r^3 = S$$

Both face-centered cubic (FCC) and hexagonal close packing (HCP) achieve this ratio when taken to the limit.

1.1 Upper bound

We can put an upper bound on either problem: the maximum number of spheres, $n$, for a given radius, or the maximum radius, $r$, for a given number of spheres.

$$\frac{\pi}{3\sqrt{2}} \geq \frac{nS}{V} = \frac{n^4\pi r^3}{V}$$
\[
\begin{align*}
\frac{1}{\sqrt[3]{2V}} & \geq \frac{n^4r^3}{V} \\
\frac{1}{3\sqrt{2}V} & \geq \frac{4}{3}r^3 \\
\frac{1}{4\sqrt{2}V} & \geq nr^3 \\
\text{fix } n & \text{ fix } r \\
\frac{\sqrt[3]{V}}{4\sqrt{2}n} & \geq r \\
\text{floor} \left( \frac{V}{4\sqrt{2}r^3} \right) & \geq n
\end{align*}
\]

This gives us an upperbound for either the number of spheres or the sphere radii. Note that if our packing does not allow partial spheres (spheres with part of their volume outside \( V \)) then the upper bound on \( n \) is floored to the nearest integer.

In reality, for a given \( V \) there will be lots of open spaces \(< S\) along the boundary of \( V, \partial V \). Places which FCC or HCP could not place an entire sphere, but would have been covered by a partial sphere in the respective packing scheme. So typically

\[
\sqrt[3]{\frac{V}{4\sqrt{2}n}} > r
\]

or

\[
\text{floor} \left( \frac{V}{4\sqrt{2}r^3} \right) > n
\]

The ratio of this lost volume, \( V_{\partial V} \), to the total volume, \( V \), or the packing volume, \( nS \), vanishes as \( n \to \infty \) or \( r \to 0 \). We may also notice, that if we fix \( V \), then as \( n \to \infty \) or \( r \to 0 \), the actual achieved ratio, \( \rho = \frac{n^4r^3}{V} \), converges to the maximum possible ratio: \( \rho \to \rho_{\text{max}} \).

### 1.2 Target volumes

The convergence of the achieved packing ratio to the maxium packing ratio depends and the achieved values of \( n \) and \( r \) compared to the upper bounds presented above depends heavily on the shape of the volume being packed. For values of \( r \) and \( n \) which are respectively large when considering a target volume, \( V \), the packing schemes FCC and HCP may not be the most efficient. For a toy example consider the volume that is a peanut (see Figure 1)
Figure 1: A peanut volume in 3D viewed from the side.

Figure 2: FCC or HCP can only pack a single sphere into the peanut, shown in green. About half the volume of the peanut is lost volume, $V_{\partial V}$, shown where the red overlaps the blue.

Figure 3: In this toy example, it is easy to see that for this radius the maximal packing can be achieved with two spheres. For more complicated volumes or values of $n$ or $r$, this will certainly not be so obvious.

Figure 4: By reducing the radii of the spheres packed with HCP, we may not necessarily reduce the lost volume, $V_{\partial V}$, shown where the red overlaps the blue, but we have increased the packing volume, shown in green.

Figure 5: Continuing to reduce the radii, we can see that the lost volume will converge to zero as the packing ratio converges to ideal packing ratio of HCP.
stretched in such a way that neither HCP nor FCC would place two spheres perfectly inside the peanut (see Figure 2).

But just placing two spheres one at a time in either side of the peanut would achieve a much higher ratio (see Figure 3). Now notice that as the radii of the spheres decrease the FCC and HCP packing strategies will quickly recover this lost volume, $V_{\partial V}$, mentioned above (see Figures 4 and 5). It seems to determine the true maximal values for $n$ or $r$ given a volume $V$, it would be necessary to determine this lost volume, $V_{\partial V}$, for the packing scheme in question. Then using the upper bounds mentioned above you could determine actual values for $n$ or $r$. This lost volume, $V_{\partial V}$, will defer depending on the shape of $V$, the packing scheme, and $n$ and $r$.

1.3 Convergence

We’ve shown that as $n \to \infty$ or $r \to 0$ the packing ratio must converge to the ideal packing ratio of the scheme. This is not to say that convergence is monotonic or at all smooth.\footnote{This also means that our upper bounds are not \textit{true} upper bounds. They are upper bounds in the sense that they assume the maximum possible packing ratio for any volume is the same as the average packing ratio for an unbounded volume. Certainly is the case for convex shapes when $r$ is small compared to $V$. The following example shows an extreme case where the upper bounds would not hold.} Especifly if we do not allow partial spheres, then the packing ratio approaches the ideal packing ratio jaggedly. Typically this means that the packing ratios achieved as $n \to \infty$ or $r \to 0$ bounce between values $< \rho_{max}$, occasionally hitting especially bad ratios, but overall improving toward $\rho_{max}$.

It is possible in some cases that the packing ratio achieved for certain values of $n$ or $r$ is higher that $\rho_{max}$, and could even be perfect: i.e. $\rho = 1.0$.

To show this, imagine that the volume we are trying to packing is exactly the volume of 4 spheres packed using HCP with radius 1 (see Figure 6). So, a properly aligned HCP of 4 spheres with radius 1 will achieved perfect packing of this volume (see Figure 7).

As $n \to \infty$ or $r \to 0$, this perfect packing will never again be reached, since with any other combination of $n$ and $r$ there must be some lost volume, $V_{\partial V}$, along the boundary (see Figure 8). The ratio instead approaches the ideal ratio of HCP, $\rho_{max} = \frac{\pi}{3\sqrt{2}}$ (see Figure 9).

1.4 Conclusion

So in conclusion, we have a closed form for the upper bound on the number of spheres, $n$, given a volume, $V$, and radii, $r$, and also a closed form for the
Figure 6: In this example, the target volume is defined to be the volume spanned by four spheres of unit radius packed according to HCP.

Figure 7: By definition of the target volume, an HCP with unit radius fill the volume perfectly with 4 spheres, achieving packing ratio $\rho = 1$.

Figure 8: Packing this volume, using HCP with other values of $n$ and $r$ cannot achieve perfect packing as there is lost volume, $V_{\partial V}$. 
upper bound on the radii, $r$, given a volume, $V$, and number of spheres, $n$. Determining which combinations of $r$ and $n$ are actually achievable depends on the volume. We’ve seen that certain volumes could have high packing ratios for large spheres, but not when conforming to HCP or FCC. We’ve also seen that for certain volumes, special combinations of $n$ and $r$ in HCP or FCC can achieve much higher ratios than even the ideal case when $n \to \infty$ or $r \to 0$. Without a closed form for the lost volume, $V_{\partial V}$, along the boundary of a given volume, it does not seem possible to have a closed form for the finding the max achievable values of $n$ or $r$ for their respective problems. The closed form for $V_{\partial V}$, unlike that for the upper bounds, would necessarily depend on the shape of $V$ not just its magnitude. In addition, the value of $V_{\partial V}$ would necessarily depend on the packing scheme used, and the values of $n$ and $r$. 

Figure 9: Instead, as $n \to \infty$ and $r \to 0$ the packing ratio converges to the ideal packing ratio of HCP.