What is the most efficient way to pack spheres inside a cuboid?

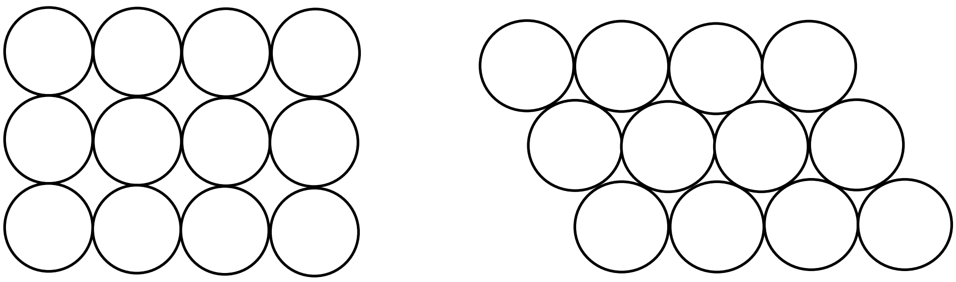
Mathematical patterns can be found everywhere, especially symmetry. The mathematical study of packing spheres is essentially the study of symmetry of spheres and looking for the highest packing density. Packing density refers to the ratio between area or volume to the area or the volume of the container. Therefore, I assume that the best way is always a uniform packing, rather than a random packing, because random packing cannot be predicted mathematically. Also, for packing in three dimensions, C.A. Rogers showed that the maximum packing density (η) satisfies[1]:

$$\eta_{max}=3\sqrt{2}(\cos^{-1}\frac{1}{3}-\frac{\pi}{3})\approx 0.77963557$$

And only uniform packings have been shown that has the closest packing density to that. Spheres are in three dimensions, so it will be easier if we start investigating in two dimensions.

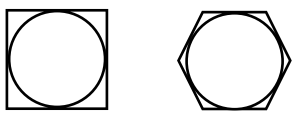
Circle Packing

In two dimensions, there are two major ways to pack circles:



Rectangle packing (Figure 1.1) Hexagonal packing

The reason why this is called rectangle packing is because if we add in the tangents to figure 1.1 and pick one circle as an example each, it will look like:



(Figure 1.2)

And now it is easy to calculate the packing density. Let the circles' radius be 1 unit.

For rectangle packing, $\eta=\frac{area\ of\ circle}{area\ of\ square}=\frac{\pi}{4}\approx 0.7854$

For hexagonal packing, $\eta=\frac{area\ of\ circle}{area\ of\ hexagon}=\frac{\pi}{2\sqrt{3}}\approx 0.9069$

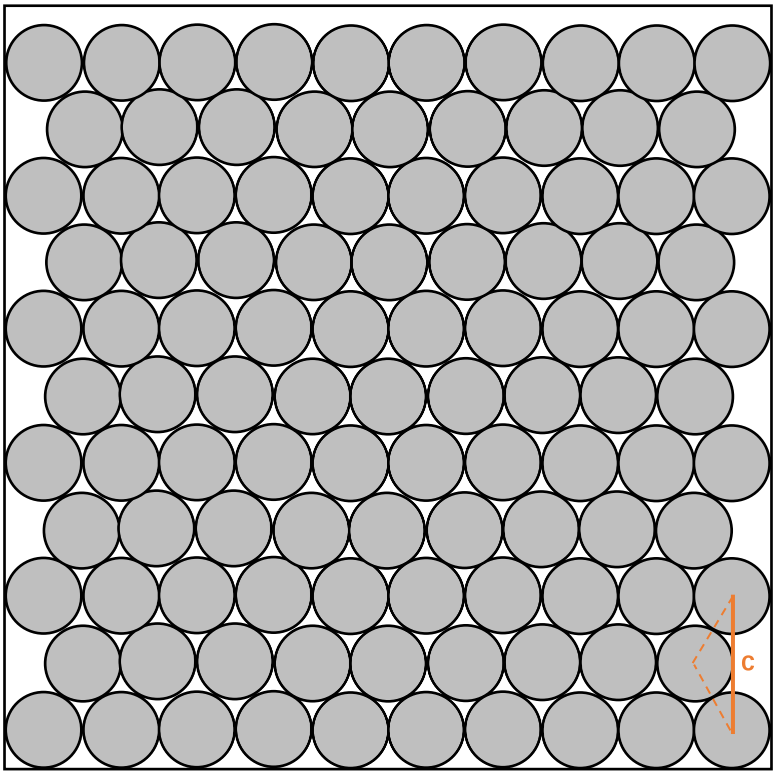
1. Sphere packing, WolframMathworld;

It is obvious to see that hexagonal packing has a much higher packing density, but doesn't mean we should always use hexagonal packing. Here is an example[2]:

Question: What is the greatest number of balls of diameter 1 that can be placed in an $10 \times 10 \times 1$ box?

Solution: This question may look like a 3D problem, but it can actually be solved in 2D. We basically try to find what is the greatest number of circles of diameter 1 that can be placed in an 10×10 square.

We start with paving a 10×10 grid with hexagonal packing.



(Figure 1.3)

After we have done 6 rows of 10 circles and 5 rows of 9 circles, which is **105** circles in total, we can't fill in any more rows. However, we can find there are some gaps at the top. The total height(H) we have done can be represented as:

$$H = 5c + d$$

Where c is the height of each hexagon minus one diameter of the circle and d is the diameter of the circle which is 1.

The height c can be found by using cosine rule:

$$c^2 = 1^2 + 1^2 - 2 \times \cos 120° \Rightarrow c = \sqrt{3}$$

Therefore, $$H = 5 \times \sqrt{3} + 1 \approx 9.66$$

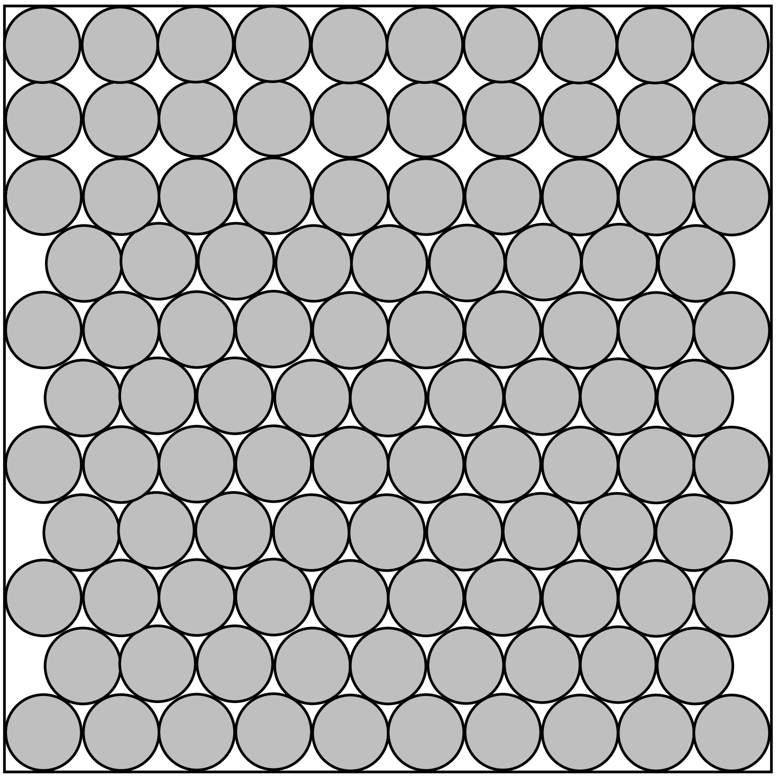
2. Sphere packing, Brilliant;

Which means we have approximately 10-9.66=0.34 left vertically. Then the idea would be to improve the gap at the top. If we take off the top two rows, H becomes

$$H = 4 \times \sqrt{3} + 1 \approx 7.928$$

We can see that the height left is approx. 2.072, and it is bigger than 2. Which means we can fill in 2 rows of ten circles because the height for rectangle packing is 1. Although the rectangle packing is less vertically efficient, it is horizontally more efficient (always 10 circles each row).

So, it will now look like:



(Figure 1.4)

Now we have 7 rows of 10 circles and 4 rows of 9 circles. The total number of rows remains 11, but now we have 106 discs.

$$H = 4c + 3d = 4 \times \sqrt{3} + 3 \approx 9.928 \implies 10 - H \approx 0.072$$

If we want to add another row of hexagon packing, then the extra height requiring(h) is

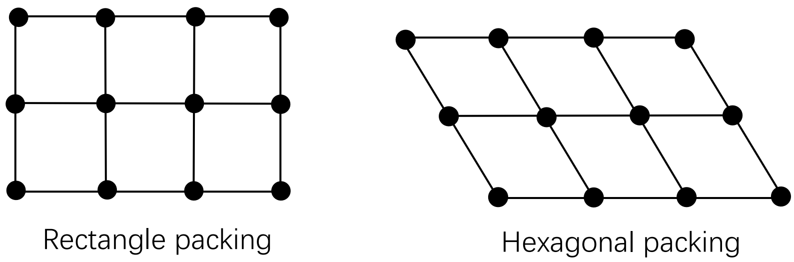
$$h = \frac{\sqrt{3}}{2} - \frac{1}{2} \approx 0.366 > 0.072$$

which shows that this is the best way we can do by using this method.
From this approach, we conclude the answer should be **106** spheres.

This is a great example to show that we need to be flexible about this kind of questions and the strategy to combine different packings can also be used in 3D sphere packing. Additionally, the packing density in 2D in this problem is approximately 0.833 and packing density in 3D is approximately 0.555.

Before we move on to 3D, we need to be able to understand what is meant by lattice structure. This is because some diagrams look really complicated in 3D, where a simple lattice structure will look a lot nicer. Let's define the centre of the circle/sphere as the lattice points because these points are all equally spaced.[3] We can extract the major lattice structures of 2D packing from figure 1.1.

Note: ● *denotes a lattice point and '—' indicates which circles/spheres are connected to each other.*

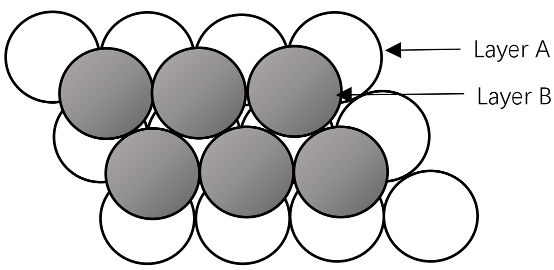


(Figure 1.5)

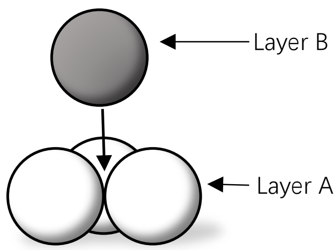
Figure 1.5 illustrates the lattice structures from figure 1.1. The all have 12 lattice points, and they all have 4 points at each row, so I call this kind of structure "4×3". It is obvious that the left "4×3" has a greater height then the right one, but has a smaller width than the other one, which shows the rectangle packing is more horizontal efficient but less vertical efficient than the hexagonal packing. That's the advantage of using lattice structure because we can identify some properties straight away.

Sphere Packing

As we have pointed out above, hexagonal packing of a single layer has a higher packing density than rectangle packing, so this is where we begin. Imagine we place the first layer at bottom. We call this layer A. Then we need to put the second layer (grey) on top of layer A. To maximize the packing density at each layer, the second layer should be hexagonal packed (figure 1.6), we would expect the spheres of new layer nestle in the hollows of layer A as demonstrated in figure 1.7.



(Figure 1.6)



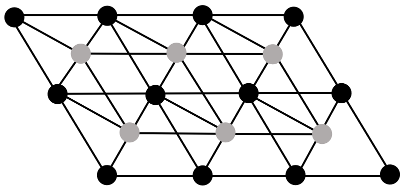
(Figure 1.7)

3. 7.8: Cubic Lattices and Close Packing, Chemistry LibreText;

There should be two ways to construct layer B in figure 1.6, the only difference is which hollows vertexes the second layer choose to touch with the first layer, but the packing density is completely the same, so I will carry on using figure 1.6 in the rest of this report.

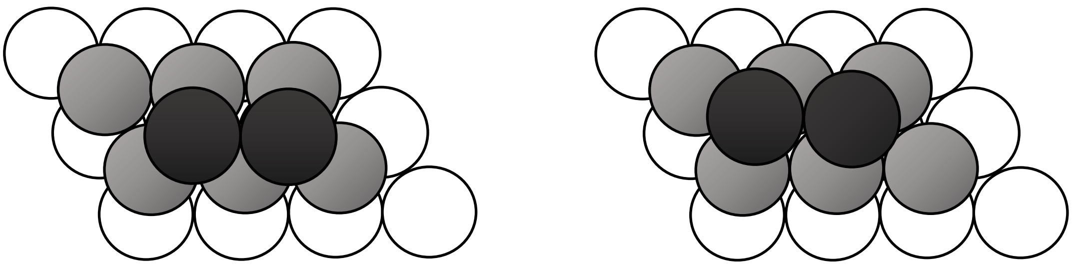
At this stage the lattice structure will look like as shown in figure 1.8.

Note: ● *denotes the lattice points of layer B.*



(Figure 1.8)

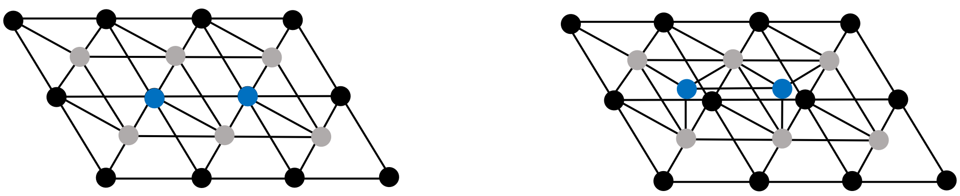
Now consider what will happen if we lay down a third layer. Again, the spheres in the third layer should be placed into the hollows within the layer B. There will be two ways of packing. However, unlike what we have discussed above, these two types of packing are completely different in terms of structure.



(Figure 1.9)

The spheres in the third layer are coloured in black. The lattice structure for both will look like as shown in figure 1.10.

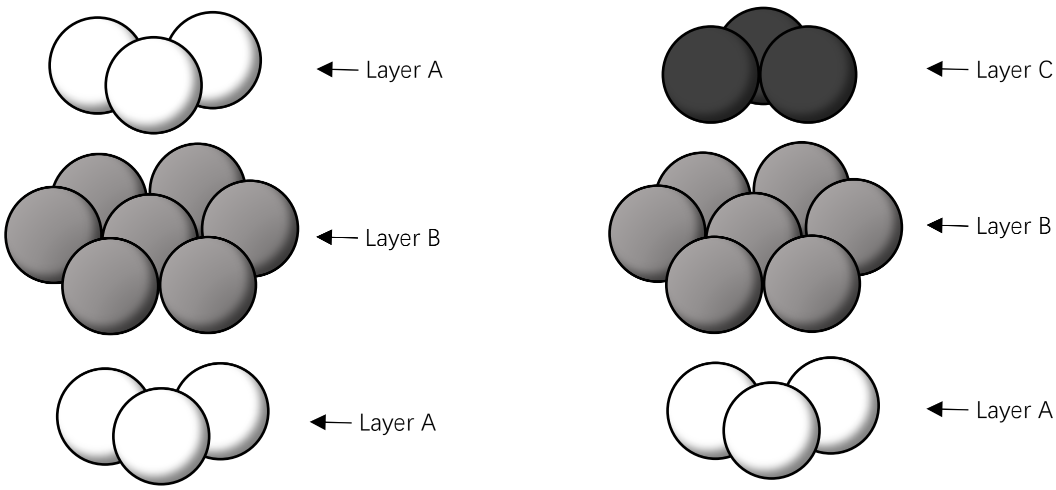
Note: ● *denotes the lattice points in the third layer.*



(Figure 1.10)

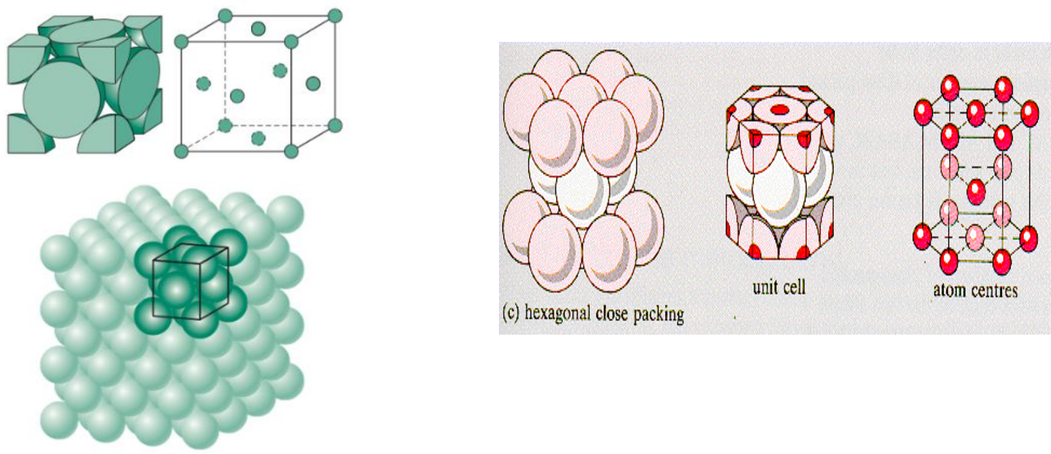
As shown in figure 1.10, the lattice points on the left structure have covered some of the lattice points of layer A, which means spheres within the third layer is right on top of some spheres within layer A. That suggests the third layer in this case is just layer A. Imagine if we put a forth layer on top, all spheres fill in void spaces, it will become another layer B. If we carry on, the layers form a sequence: ABABABABAB……

However, the lattice structure on the right has a completely new layer, so let's call it layer C. But now if we add more layer to layer C, also fill in the void spaces, we get another layer A. If we carry on repeating adding a new layer, the layers form another sequence: ABCABCABC……



"ABABAB…" (Figure 1.11) "ABCABC…"

We name "ABABAB……" as hexagonal close packing (HCP) and "ABCABC……" as cubic close packing (or face centered cubic, FCC).[4] [5] But many layers of stacking are possible, for example ABAC, ABCC, BACA…… Depends on particular cases, we may need to use the strategy we were talking about earlier to assemble different layers.



(Figure 1.12 showing the unit cell, lattice structure from side and an overall looking of both packings.)

From unit cell of each packing which has been shown in figure 1.12, we can now easily calculate each packing's packing density:

For FCC, $\eta = \frac{volume\ of\ all\ spheres}{volume\ of\ unit\ cell} = \frac{\pi}{3\sqrt{2}} \approx 0.7408$

4. Face Cantered Cubic, PennState College of Earth and Mineral Science

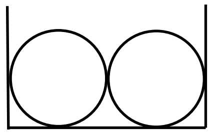
5. Newey and Weaver, "Materials Principles and Practice," Butterworth (1990)

For HCP, $\eta = \frac{volume\ of\ all\ spheres}{volume\ of\ unit\ cell} = \frac{\pi}{3\sqrt{2}} \approx 0.7408$

It is amazing to see that two different structures have exactly same packing density with different structure. This gives us a great flexibility to assemble different layers. Now I am going to show how to apply these techniques.

Practical Modeling

I am going to try to model the most efficient way of packing spheres using Python (version 3.6.4). But my program will only work when the cuboid's width divides the diameter of spheres is an integer, in the other word: $\frac{the\ width\ of\ the\ cuboid}{the\ diameter\ of\ sphheres} \in \mathbb{Z}^+$, where $\mathbb{Z}^+$ denotes the set of positive integers. The reason is because when the proportion is an integer, the optimal number of circles/spheres in a row would always be $\frac{the\ width\ of\ the\ cubic\ object}{the\ diameter\ of\ sphheres}$ (as shown in figure 1.13) and we only need to think about to optimal solution for other dimensions.



(Figure 1.13; It shows a rectangle with a width of 2 unit and circles with diameter to be 1 unit. And this must be the optimal solution in horizontal direction which it is the same direction as width.)

This makes the modelling more doable because different dimensions are perpendicular to each other at different planes and we don't have an optimal solution for inclined directions between each two planes so the uncertainty is too huge which it is not good for finding a fixed general solution.

Although HCP and FCC has same packing density, in terms of height they are different:

height of one HCP unit cell: $\frac{2\sqrt{6}}{3}d \approx 1.633d$

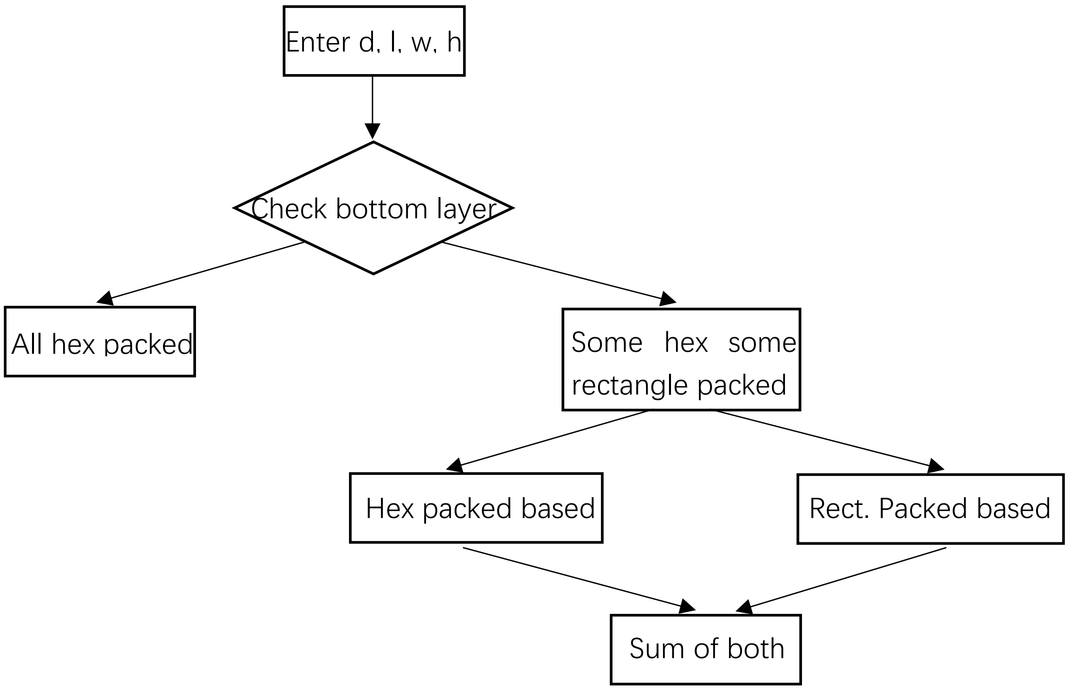
height of one FCC unit cell: $\sqrt{2}d \approx 1.414d$

"d" represents the diameter of the sphere. We can see that for the same spheres, FCC is more vertically efficient than HCP. It indicates that the program should always consider FCC first rather than HCP.

Now imagine we have a $l \times w \times h$ cubic object (l=length, w=width, h=height) and spheres of d diameter, where $\frac{l}{d} \in \mathbb{Z}^+$.

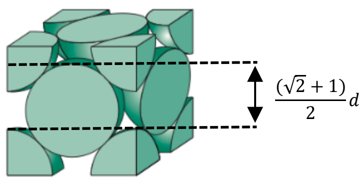
First, we need to find an optimal solution for the first layer which is a $l \times w \times d$ three-dimension space or we can treat it as a $l \times w$ two-dimension plane. Because this report is mainly about sphere packing, so I am not going to talk too much about it but the idea is similar to what I have talked about in "Circle Packing". For the actual code, please see "2D-circle packing.py".

Now we will either have first layer with all hexagonal packed spheres (E.g. figure 1.3) or some hexagonal packed spheres with some rectangle packed spheres (E.g. figure 1.4). The strategy is shown in figure 1.14.



(Figure 1.14)

For all hexagonal packed spheres, we will try FCC first. One period of FCC is made up by a sequence "ABC", which has a height of $(\sqrt{2}+1)d$. Thus, the number of period the object can do (n) equals $\lfloor\frac{h}{(\sqrt{2}+1)d}\rfloor$, where ⌊⌋ is called floor function which only takes the integer part of the result, E.g. ⌊2.71⌋=2. The gap left(g) will be $(\mathrm{h}-\mathrm{n}\times(\sqrt{2}+1)d)$. If the gap left doesn't equal to zero, we know need to check if we can fit more layers in g. Layer A/B/C all require an extra height (u) of $\frac{(\sqrt{2}+1)}{2}d$, as shown in figure1.15.



(Figure 1.15)

Now there are three possible cases:

1. $\left\lfloor\frac{g}{u}\right\rfloor = 0$, this is when $u > g$, the arrangement for the layers would be a rotation of "ABC" for n times.
2. $\left\lfloor\frac{g}{u}\right\rfloor = 1$, this is when $u > \frac{g}{2}$, the arrangement for the layers would be a rotation of "ABC" for n time plus a layer A.
3. $\left\lfloor\frac{g}{u}\right\rfloor = 2$, this is when $u \leq \frac{g}{2}$, the arrangement for the layers would be a rotation of "ABC" for n times plus "AB", which is a HCP packing.

We need to find out how many spheres are in each layer. As I have mentioned before, the number of spheres in layer A has been solved, so we only need to find layer B&C. As we can see in figure1.3, the bottom row(row A) should always start with $\frac{l}{d}$ number of spheres in layer A, and the row above(row B) should always be $\frac{l}{d} - 1$ number of spheres, other rows just repeat this pattern. In row A we can see that there is a hollow between two touched spheres, and each hollow means we can put a layer B sphere there. Therefore, we can put $\frac{l}{d} - 1$ number of layer B spheres, and it is the same for row B. So, in total, we can put $\left(\frac{l}{d} - 1\right) + (\frac{l}{d} - 2)$ layer B spheres which equals $\frac{2l}{d} - 3$ layer B spheres. Because this pattern is repeated, then we only need count how many times it has repeated and we get our general formula:

$$\boldsymbol{num. of\ spheres\ in\ layer\ B = min\ (num. of\ row\ A, num. of\ row\ B)} \times (\boldsymbol{\frac{2l}{d} - 3})$$

Note: *min (A, B) means take the smaller one between A and B. E.g. min (2, 5) = 2.*

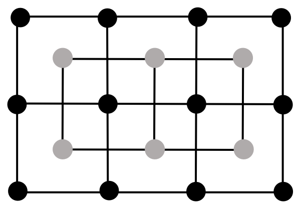
For the number of spheres in layer C, it is the same idea as before. Let the bottom row in layer B to be row C, it has $\frac{l}{d} - 1$ number of spheres. The row above row C in layer B, we call it row D, it has $\frac{l}{d} - 2$ number of spheres. The number of hollows they have in total is $\frac{2l}{d} - 5$. Therefor the general formula for layer C would be:

$$\boldsymbol{num. of\ spheres\ in\ layer\ C = min\ (num. of\ row\ C, num. of\ row\ D)} \times (\boldsymbol{\frac{2l}{d} - 5})$$

Now we can easily calculate the total number of spheres for three different cases.

For the cases that layer A is partly rectangle packed the idea is to nestle spheres into the hollows as demonstrated in figure 1.16:

Note: ● *denotes the lattice points of layer A.* ● *denotes the lattice points of layer B.*



(Figure 1.16)

Layer C will be right on top of layer A, so it is just simply a rotation of “AB”. The general formula for the number of spheres in one “AB” is:

$$\boldsymbol{num. of\ spheres\ in}\ \mathrm{AB} = (\boldsymbol{num. of\ row\ A - 1}) \times (\boldsymbol{\frac{l}{d} - 1})$$

The number of period it can do (n) is $\left\lfloor\frac{2h}{(\sqrt{3}+1)d}\right\rfloor$. The gap left ($g$) equals $(\mathrm{h} - \mathrm{n} \times \frac{(\sqrt{3}+1)d}{2})$. The extra height for another layer B (u) is $\frac{(\sqrt{3}-1)d}{2}$. Now there are two cases:

1. $\left\lfloor\frac{g}{u}\right\rfloor = 0$, the arrangement will be a rotation of “AB” for n times.

2. $\left\lfloor \frac{g}{u} \right\rfloor = 1$, the arrangement will be a rotation of "AB" for n times plus a layer B.

The total number of spheres would be the sum of spheres above all hexagonal packed layer A and spheres above rectangle packed layer A and layer A. Please see "3D-sphere packing.py" for the coding. Here is an example of the program's interactive window:

Input:

-----Regular sphere 3D packing-----

Please enter three parameters of a cubic:

Note: Width/diameter needs to be an integer and h >= d.

Length:10

Width:10

Height:10

Diameter:1

Output:

Maximum number of spheres: 1195.0

Conclusion

For conclusion, I think I have managed to find a way to model the sphere packing in a cubic. However, my model has restrictions. Firstly, my model can only deal with $\frac{l}{d} \in \mathbb{Z}^{+}$. Secondly, my model is designed to happen under ideal concepts, such as all spheres are perfectly tangent to each other as they are only touched at one point, so this model may not work under a real-world situation.

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