Sphere Packing Lattice Generation

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1 Elements of Sphere Packing

Our goal is to take a three dimensional space and fill it with spheres. We can't fill the whole space with spheres, but certain arrangements, certain sphere packing routines minimize the empty space. Let's call our three dimensional volume which we want to fill the *box* and refer the the spheres as *balls*. All of our balls—for now—will have the same radius.

Whenever two balls touch the distance between their centers is $(r_1 + r_2)$, where r_1 is the radius of the first ball and r_2 is the radius of the second. So in our case the distance is simply $2r$. This will be helpful to remember when the geometry gets trickier: any time two balls touch the distance between their centers is $2r$.

1.1 A Tetrahedron of Balls

For a moment forget the balls and consider the regular tetrahedron, a four-faced pyramid with a triangle base.

If we place one corner of the tetrahedron on the origin and two more on the $z = 0$ plane, then we can say its base is resting on the $z = 0$ plane. Given a side length a the coordinates of the corners would be as follows:

$$(0, 0, 0), (a, 0, 0), (\frac{1}{2}a, \frac{3\sqrt{3}}{6}a, 0), (\frac{1}{2}a, \frac{\sqrt{3}}{6}a, \frac{\sqrt{6}}{3}a) \tag{1}$$

Imagine that $a = 2r$, where r is the radius of our balls, then we could place four balls so that each one's center landed on a corner of the tetrahedron. Each ball would be touching the other three balls, so we know the shape formed by their centers has to be this regular tetrahedron. If we then imagine three of the balls to be laying on a plane and the fourth ball resting on top the shape would be a familiar, simple stack of spheres. See Figure 1 on page 2.

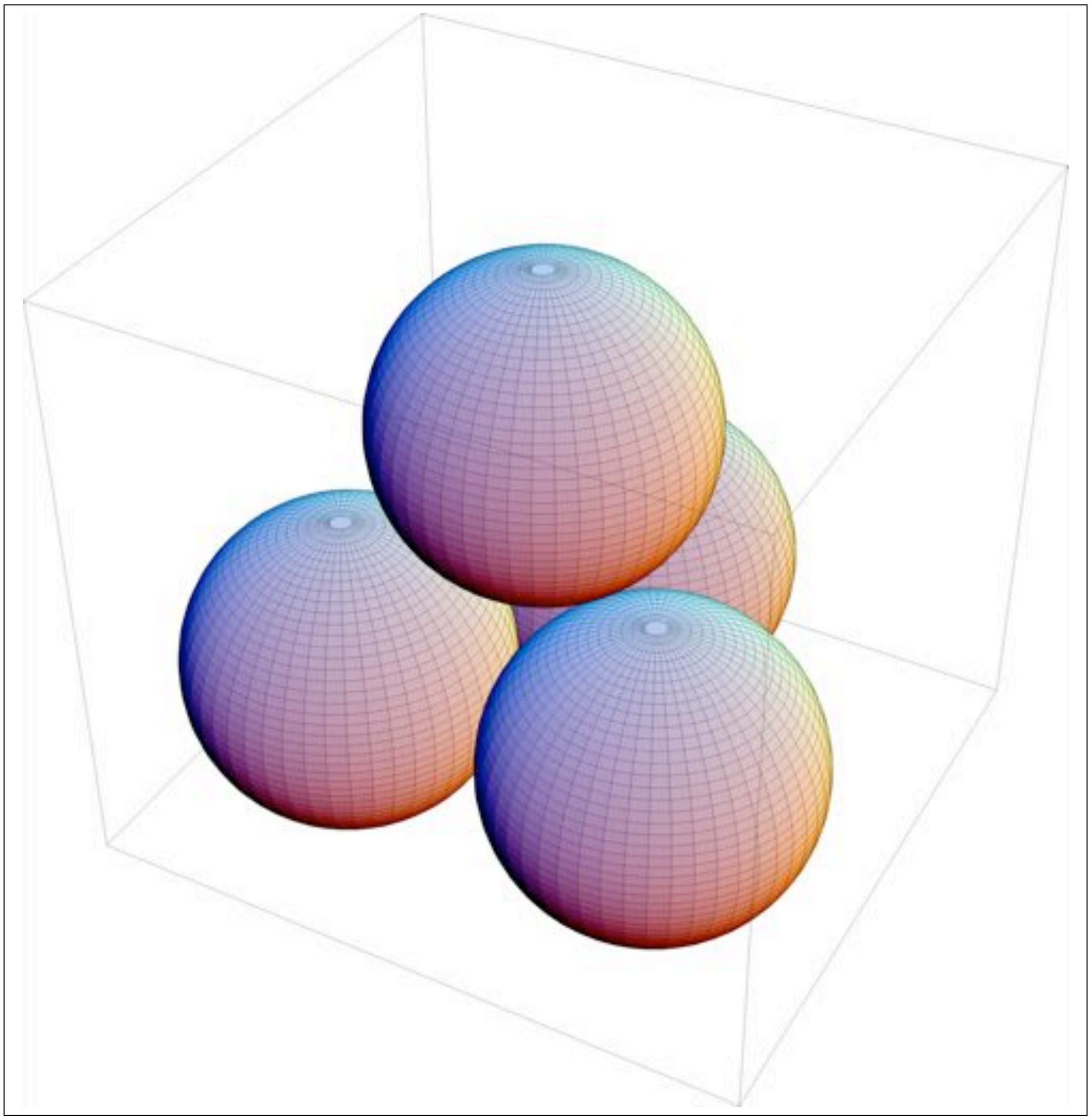

Figure 1: Regular tetrahedron of equal-radius balls

If the *base* is the three balls are resting on the $z = 0$ plane, then the center of the *top* ball, the one resting on the lower three, has a different z-coordinate than the others. The difference is the same as the height of the tetrahedron their centers form: $\sqrt{6}a/3$, where a is the side length. So in our case, the z-pitch between planes of balls is $2\sqrt{6}r/3$.

1.2 Filling a Space with Spheres

To fill the box with the most balls, we could use a Face-Centered Cubic packing routine or a Hexagonal Close-Packed packing routine. The planes fit together in certain patterns which are more efficient. FCC routines always require at least three different plane types, so a typical FCC pattern might be: A-B-C-A-B-C-A-.... See Figure 2 on page 4. There is an HCP routine that achieves maximum possible efficiency with only two plane types in a simple pattern of: A-B-A-B-A.... So while both FCC and HCP are proven to be maximally efficient packing routines, we will use this simpler HCP routine to form our lattice of the balls' centers.

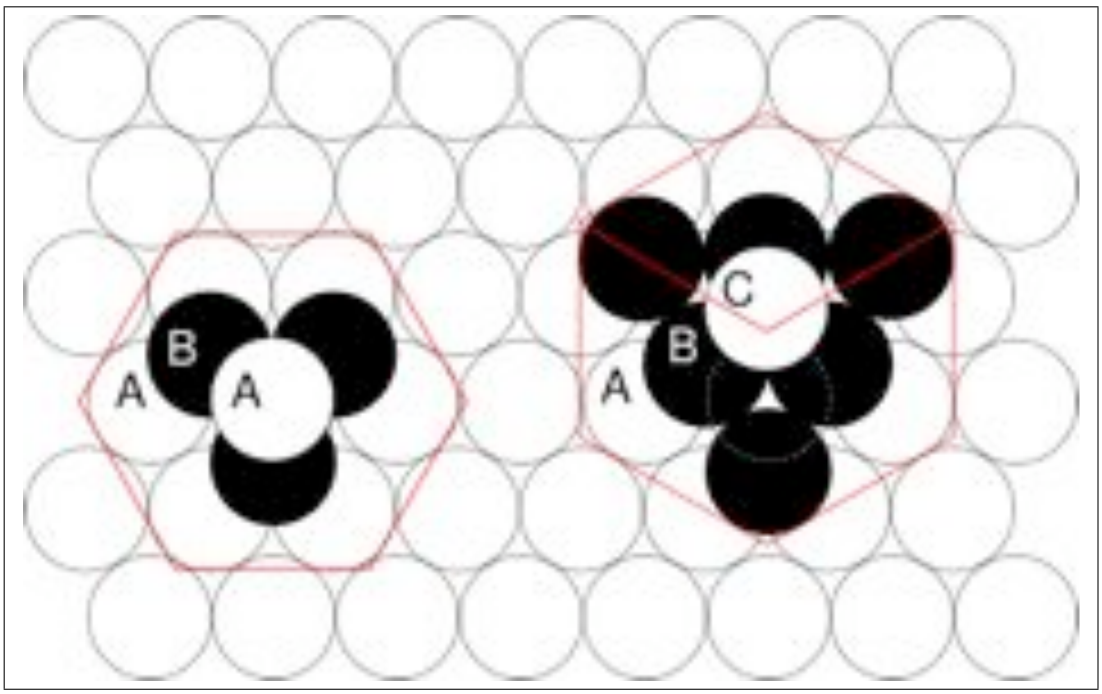

Figure 2: HCP packing routine is on the left, FCC on the right.

The result of our goal of filling the box with balls will be in the form of a lattice. Each point on the lattice will represent a center of a ball. Using the lattice, we need only to place balls so that their centers lie on a lattice point, and the box will fill.

2 Making the Lattice: Plane by Plane

2.1 The A Plane: Row by Row

For our lattice to be useful, we will want it be easily transformed and translated to fill any 3D space. So to make things easier let's have a rule that all points on our lattice will be non-negative. Therefore, our box must also contain no negative points. So, the best place for our box is with one corner at the origin and leveled with a side on each positive axis.

With an idea of what space we're trying to fill, we begin by making one row of balls. Start with a hypothetical ball centered at $(0, r, r)$ on the xyz-space with a radius, r. Some of this ball's volume will be outside the box so its center will not end up on the lattice, but we will use it as a starting point. Keeping the y- and z-coordinates the same, add another ball so that the two balls touch. Add more in this row, along this line, until the x-coordinate boundary of the box is reached. See Figure 3 on page 5.

Coordinates of the centers of the first row will look like:

$$(2r, r, r), (4r, r, r), (6r, r, r), (8r, r, r), \ldots \tag{2}$$

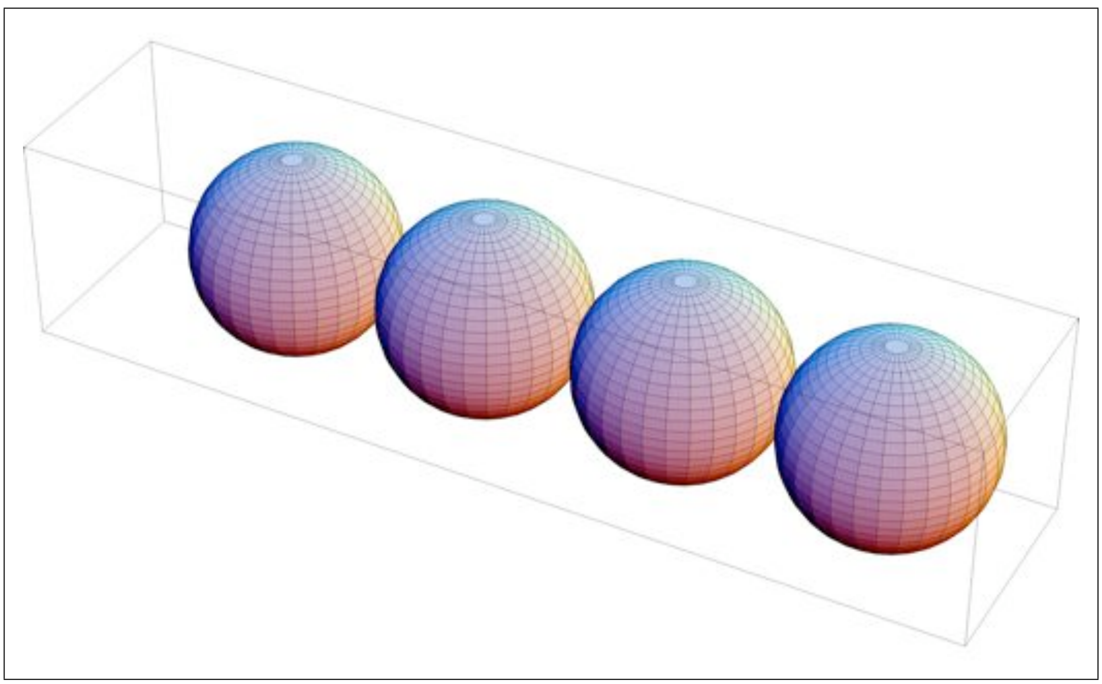

Figure 3: A row of balls, having centers with equal y- and z-coordinates.

Now we will form the next row of balls on this plane. Place a ball on the same z-coordinate plane as the first row, but with a different y-coordinate, so that it will touch the first two balls of that first row. The three centers of these balls form an equilateral triangle, the height of which is the y-pitch from the first row to the second row: $\sqrt{3}r$, because the sides of the triangle are all $2r$. The x-coordinate of the new ball is the same as the x-coordinate of the point of contact between the balls in the first row. So all the balls in the second row will have shifted a distance r. Place balls in a row with this new y-coordinate and the same z-coordinate until reaching the x-coordinate boundary of the box. See Figure 4 on page 6.

Thus, this row will have coordinates like this:

$$(r, r+\sqrt{3}r, r), (3r, r+\sqrt{3}r, r), (5r, r+\sqrt{3}r, r), (7r, r+\sqrt{3}r, r), \ldots \tag{3}$$

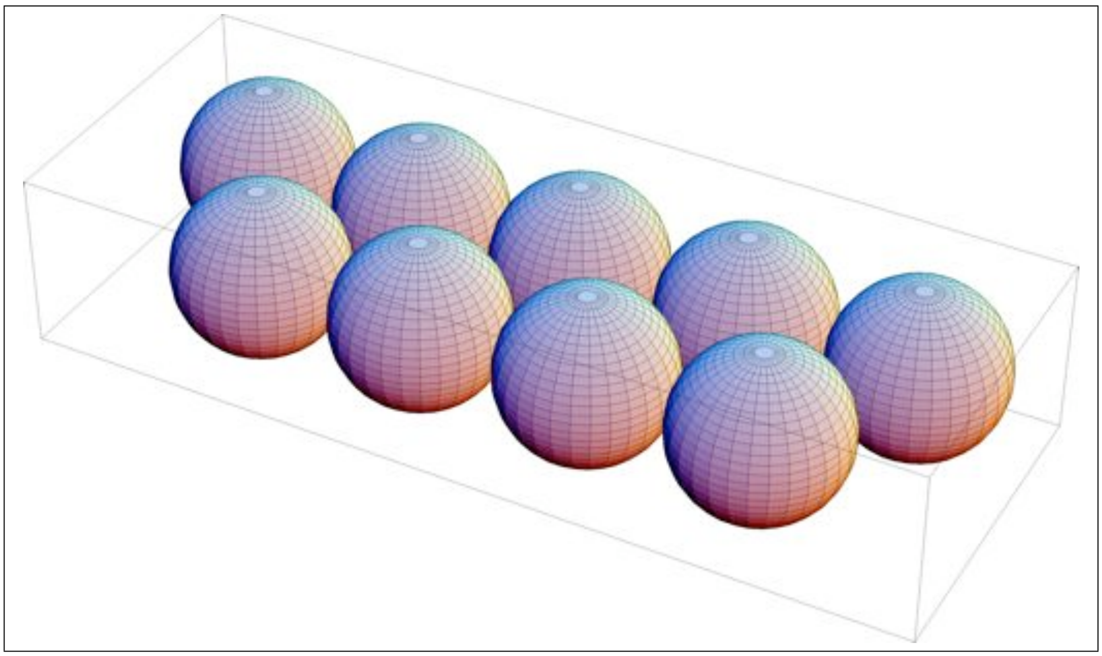

Figure 4: The first two rows of balls.

Continue this process of making new rows, by adding the y-pitch and shifting the rows in the x-direction until reaching the y-coordinate boundary of the box. This completes the A Plane of the lattice. See Figure 5 on page 6.

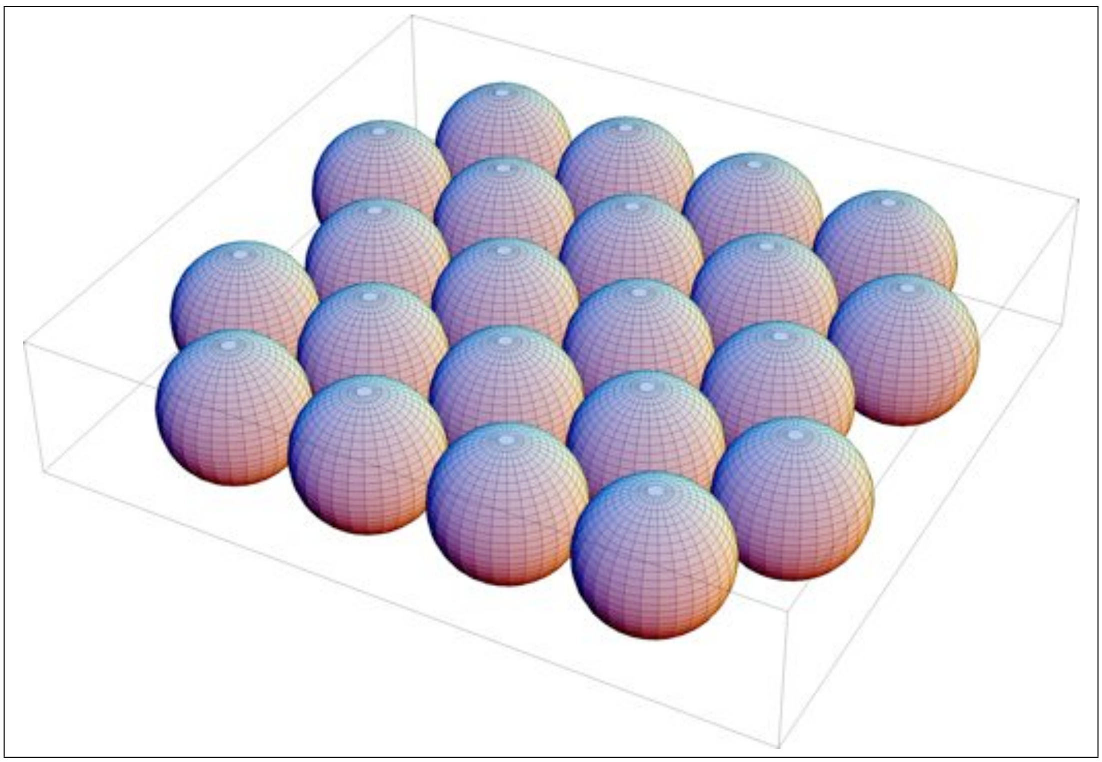

Figure 5: The first A Plane of balls.

2.2 The B Plane: Row by Row

To begin the B Plane, recall our tetrahedron made of four balls (See Figure 1 on page 2). There we placed three balls on a plane and one ball resting on top of the three. The first ball, in the first row of the B Plane will be placed just like that top ball of the tetrahedron. Place a ball on top of the three balls in the A-Plane closest to the origin. This new ball will touch all of those three balls. The difference in its z-coordinate from theirs will be the height of the tetrahedron: $2\sqrt{6}r/3$. The new balls x- and y- coordinates also follow from the regular tetrahedron. Now, keep the y- and z-coordinate of this first ball in the B Plane constant, line up balls in a row until reaching the x-coordinate boundary just like with the first row of the A Plane.

The coordinates of this row are:

$$(r, \frac{\sqrt{3}}{3}r, r+\frac{\sqrt{6}r2}{3}), (3r, \frac{\sqrt{3}}{3}r, r+\frac{\sqrt{6}r2}{3}), (5r, \frac{\sqrt{3}}{3}r, r+\frac{\sqrt{6}r2}{3}), (7r, \frac{\sqrt{3}}{3}r, r+\frac{\sqrt{6}r2}{3}), \ldots \tag{4}$$

Then proceed to make a second row on the B Plane like we did with the A Plane.

$$(2r, 2\frac{\sqrt{3}}{3}r, r+\frac{\sqrt{6}r2}{3}), (4r, 2\frac{\sqrt{3}}{3}r, r+\frac{\sqrt{6}r2}{3}), (6r, 2\frac{\sqrt{3}}{3}r, r+\frac{\sqrt{6}r2}{3}), (8r, 2\frac{\sqrt{3}}{3}r, r+\frac{\sqrt{6}r2}{3}), \ldots \tag{5}$$

Fill the B Plane with rows until again reaching the y-coordinate boundary of the box. This completes the B Plane. See Figure 6 on page 8.

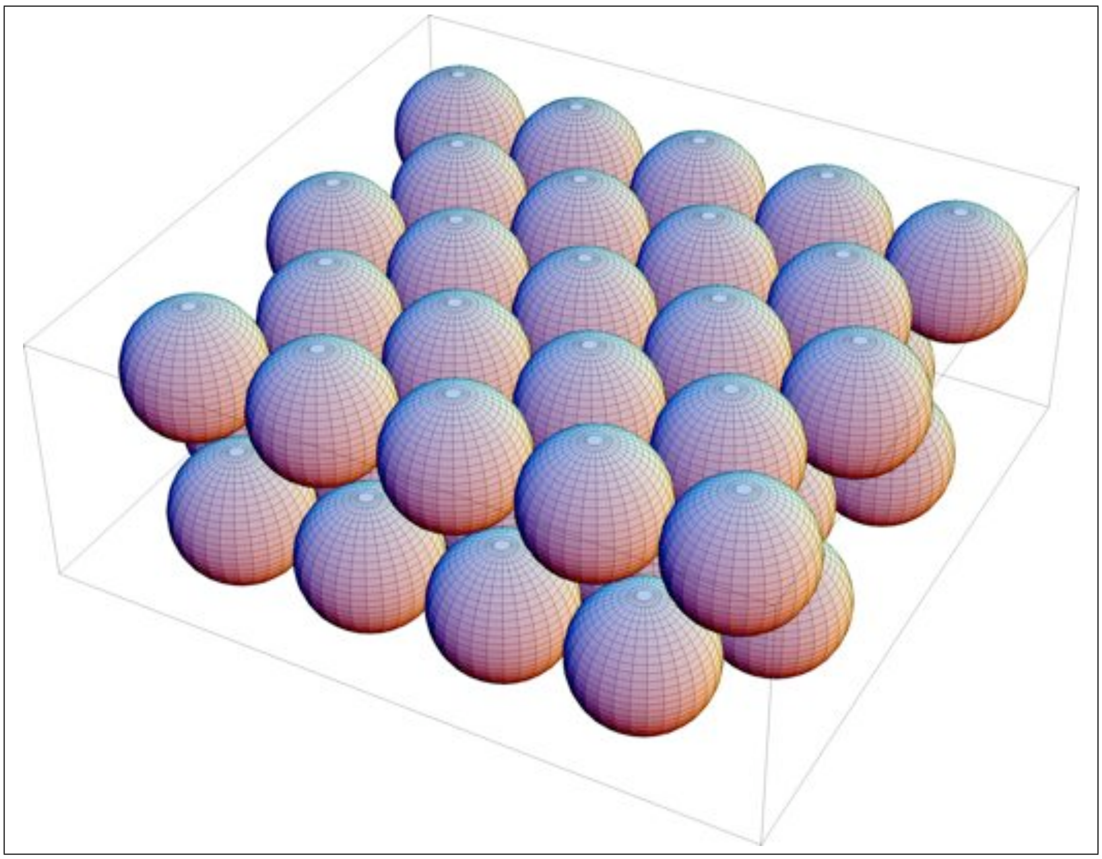

Figure 6: The first A and B Planes of balls.

2.3 Filling the Box: A-B-A-B-A-...

We have an A Plane and a B Plane. Continuing the pattern we stack an A Plane again next. The difference to the next A plane from the B Plane below, is again $\sqrt{6}r2/3$ in the z-direction. The A Plane and B Plane really refer to the x- and y-coordinates of the balls on those planes. In this second A Plane all of the balls will have the same x- and y-coordinates as the balls in the first A Plane. The z-coordinates will differ only (by two z-pitches). We can easily stack this next A Plane onto our two previous planes. See Figure 7 on page 9.

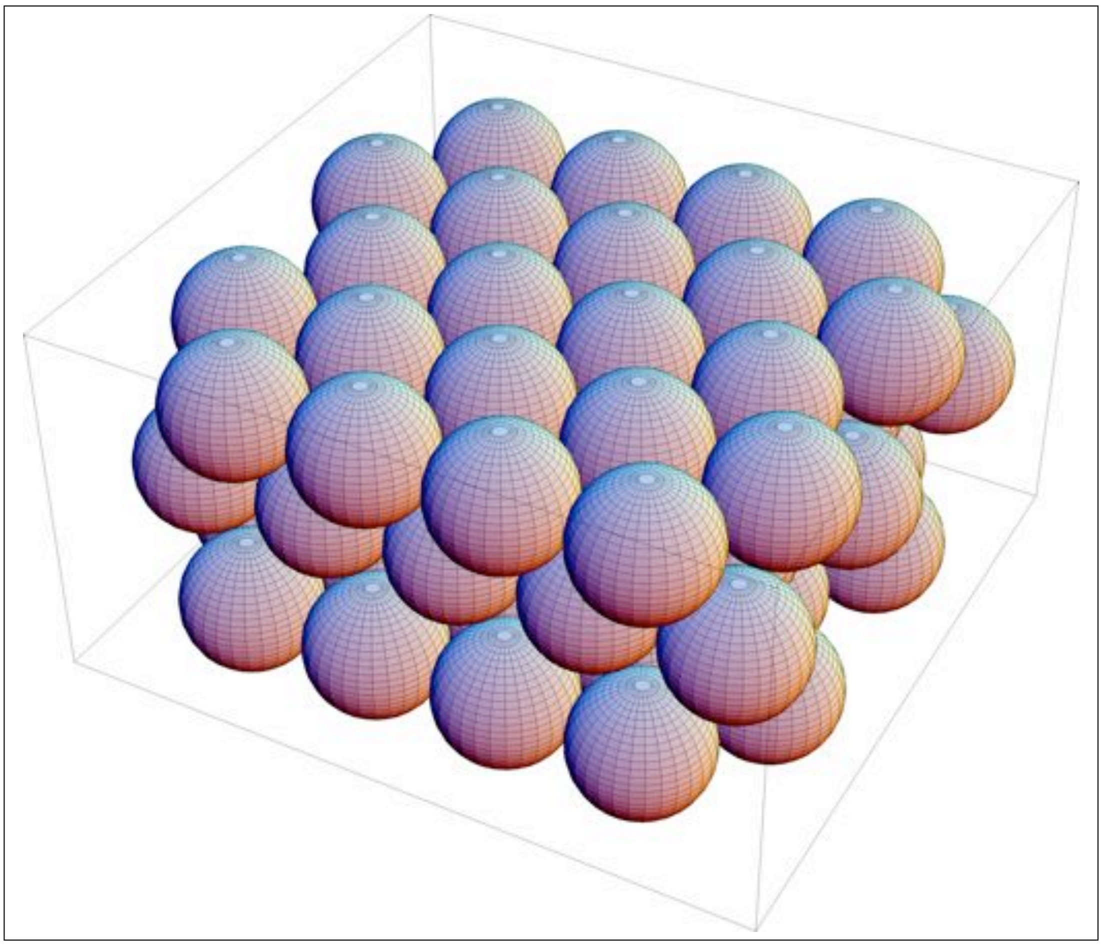

Figure 7: A second A Plane of balls is stacked onto the first two planes.

Continue stacking planes in this pattern—A-B-A-B-A-...—until reaching the z-coordinate boundary of the box. This completes the filling of the entire box. See Figure 8 on page 10.

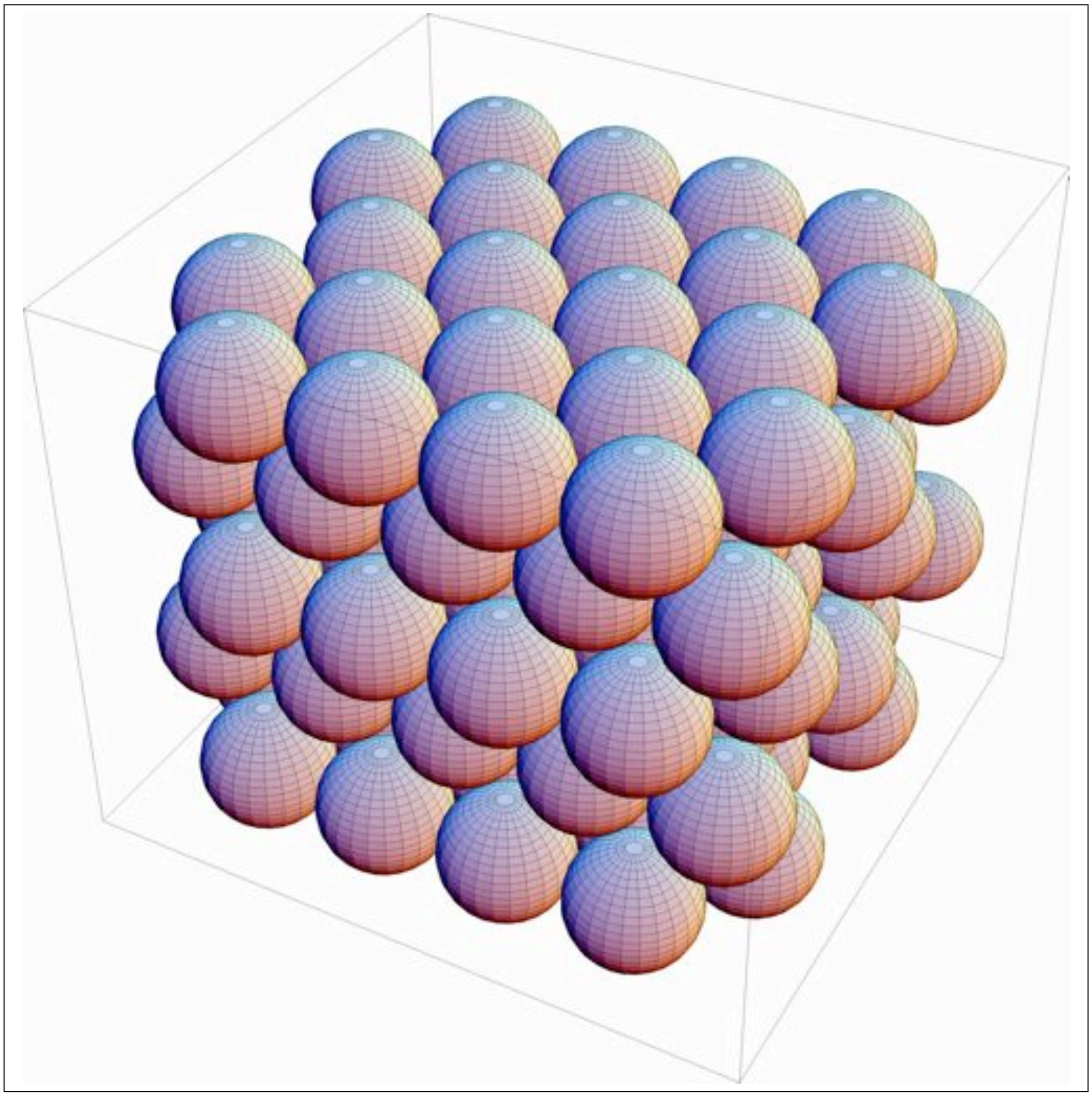

Figure 8: A box filled efficiently with balls on an A-B-A-B-A-. . . HCP lattice.

2.4 Filling the voids with smaller spheres

Every time in the A-B-A-B-A-... HCP lattice that four balls make a tetrahedron, there is a void created, centered at the center of the tetrahedron (Look closely at Figure 1 on page 2). The center of this tetrahedron is the same distance to all of its corners. So as a a tetrahedron formed of four balls, the center of the tetrahedron is the same distance to each ball's center, lattice position. The center of a tetrahedron is precisely $\frac{\sqrt{6}}{2}r$ distance from each corner. We have placed the tetrahedron in such a way—with the base on an even plane—that the coordinates of the center are the same as the coordinates of the top ball's center minus this distance. The new smaller ball hangs below the top ball. We want r', the radius of this new, smaller ball, to be maximal. So we subtract the original, larger radius from the distance to each corner: $r' = \frac{\sqrt{6}}{2}r - r -> r' = r(\frac{\sqrt{6}}{2} - 1) -> r' \approx 0.225r$. See the ball filling the void in original tetrahedron of balls in Figure 9 on page 11.

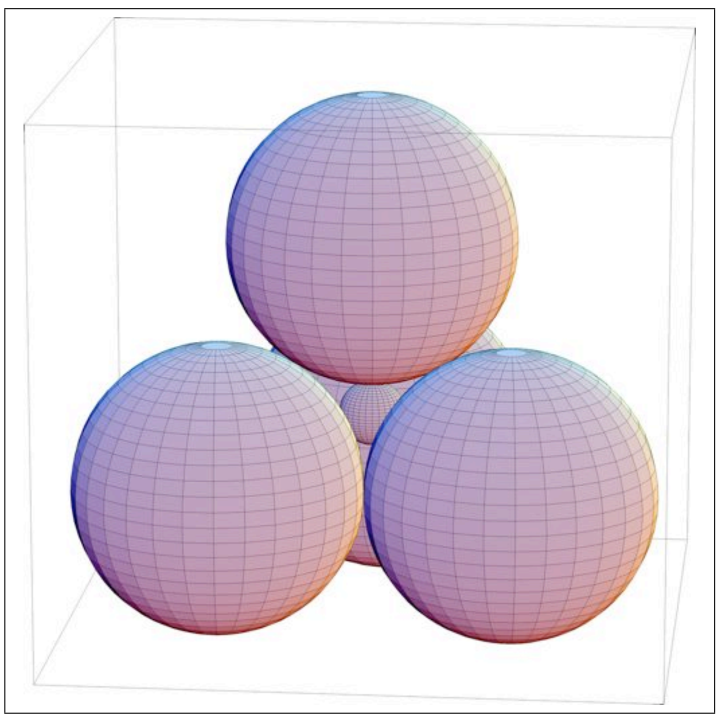

Figure 9: A tetrahedron made of balls with small ball in the void space.

To make a lattice of the centers of the new, smaller balls, we only need to modify and expand the original lattice. Every ball in the original packed box is the top ball of a tetrahedron of four balls, so we hang a small ball with radiusr' from every ball in the original lattice. But also notice that every ball is also the bottom ball of an "inverted" tetrahedron. See Figure 10 on page 12. So there also should be a new, smaller ball floating above each larger ball in the original lattice. See Figure 11 on page 13.

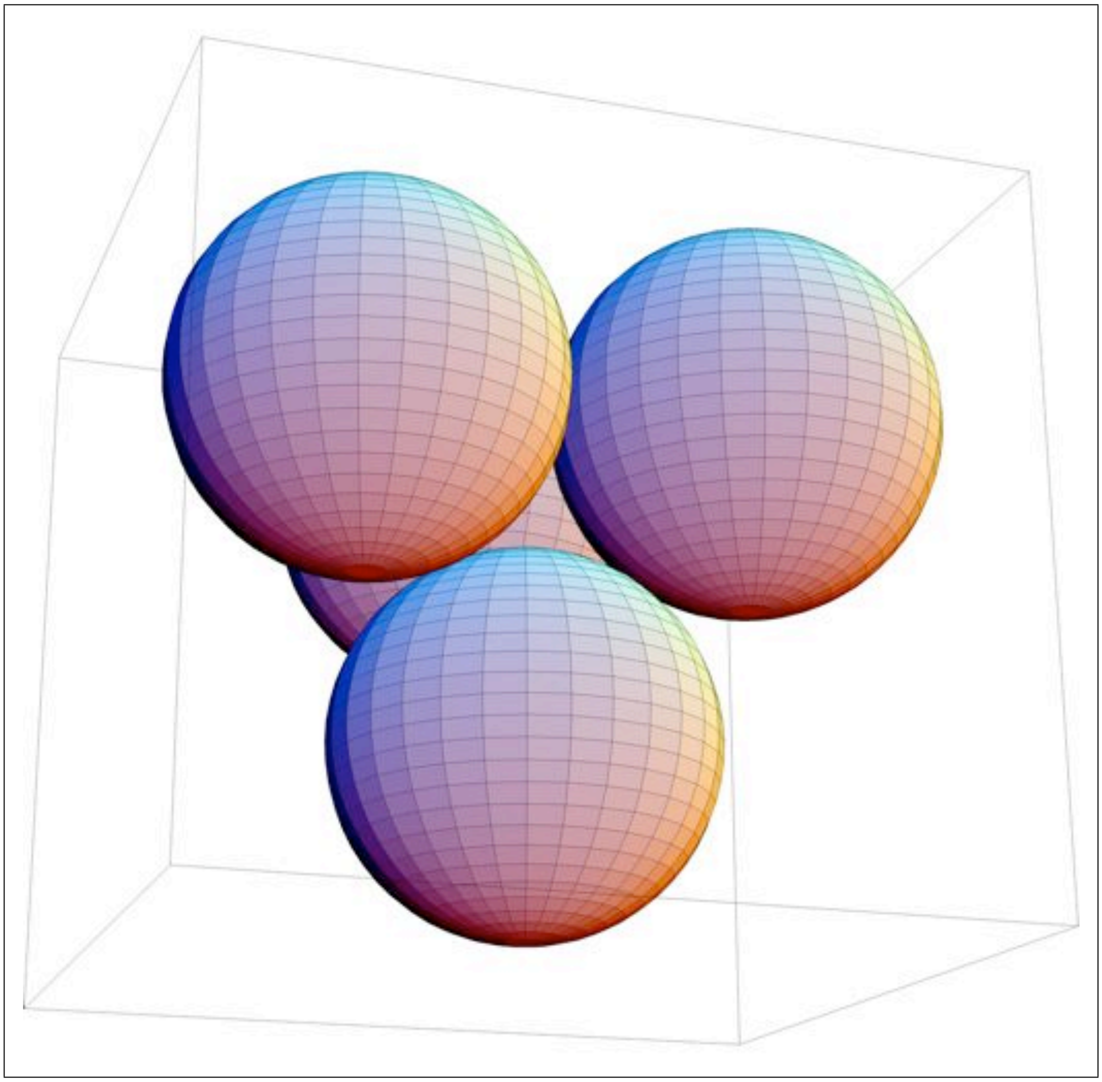

Figure 10: An “inverted” tetrahedron made of balls.

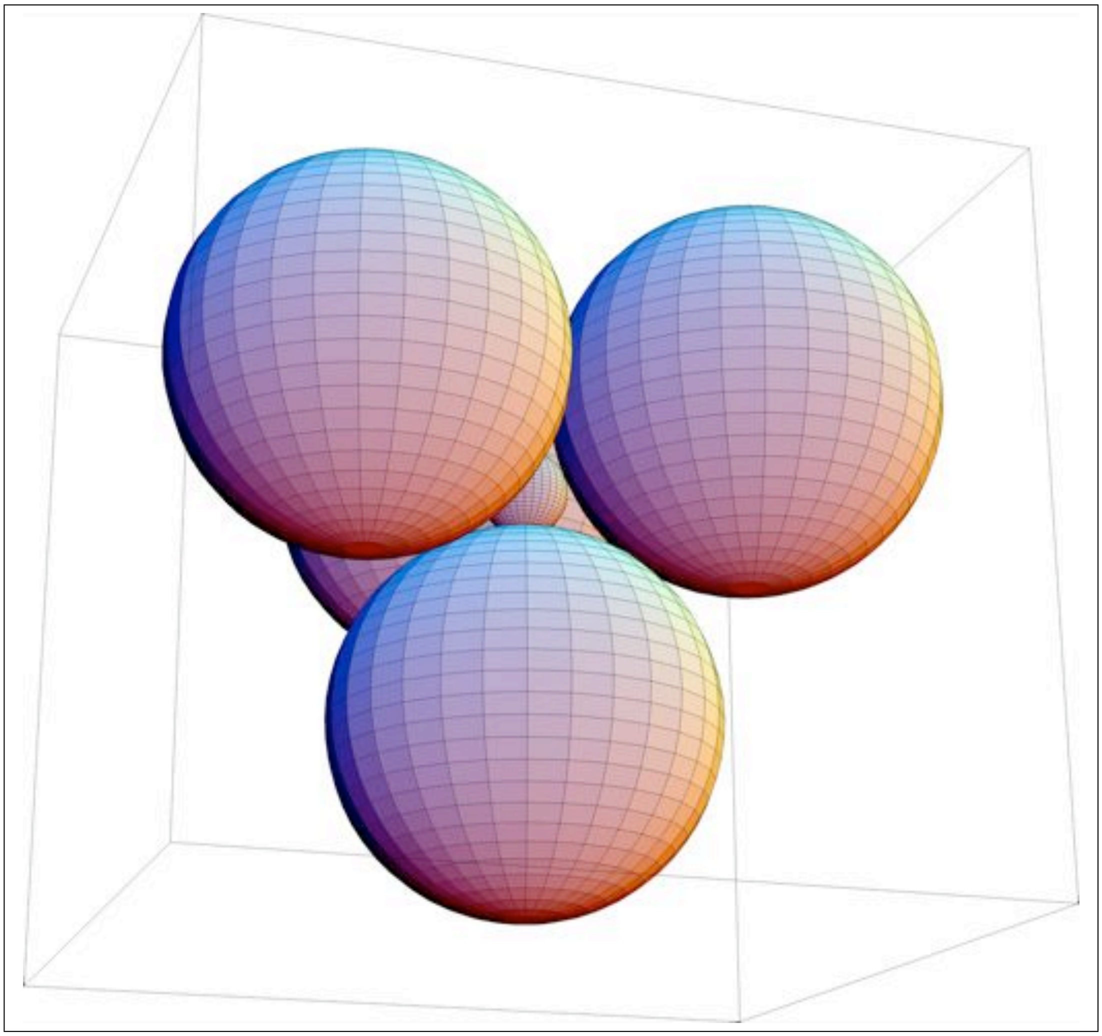

Figure 11: An “inverted” tetrahedron made of balls with small ball in void.

In an infinite space there are twice as many smaller balls as larger balls, but with a box we have boundaries. Such boundaries stopped us before from placing larger balls whose volume would partially lie outside the box. With smaller radii these new balls fit in lattice positions along the boundaries, based on balls that are technically illegal to the packing. By extending our original lattice to include these balls we can place many smaller balls along the boundaries, but still managing to maintain our strict lattice of their alignment. Look closely at Figure 12 on page 14 for the balls along the sides that have no "mother" ball to float over or hang from.

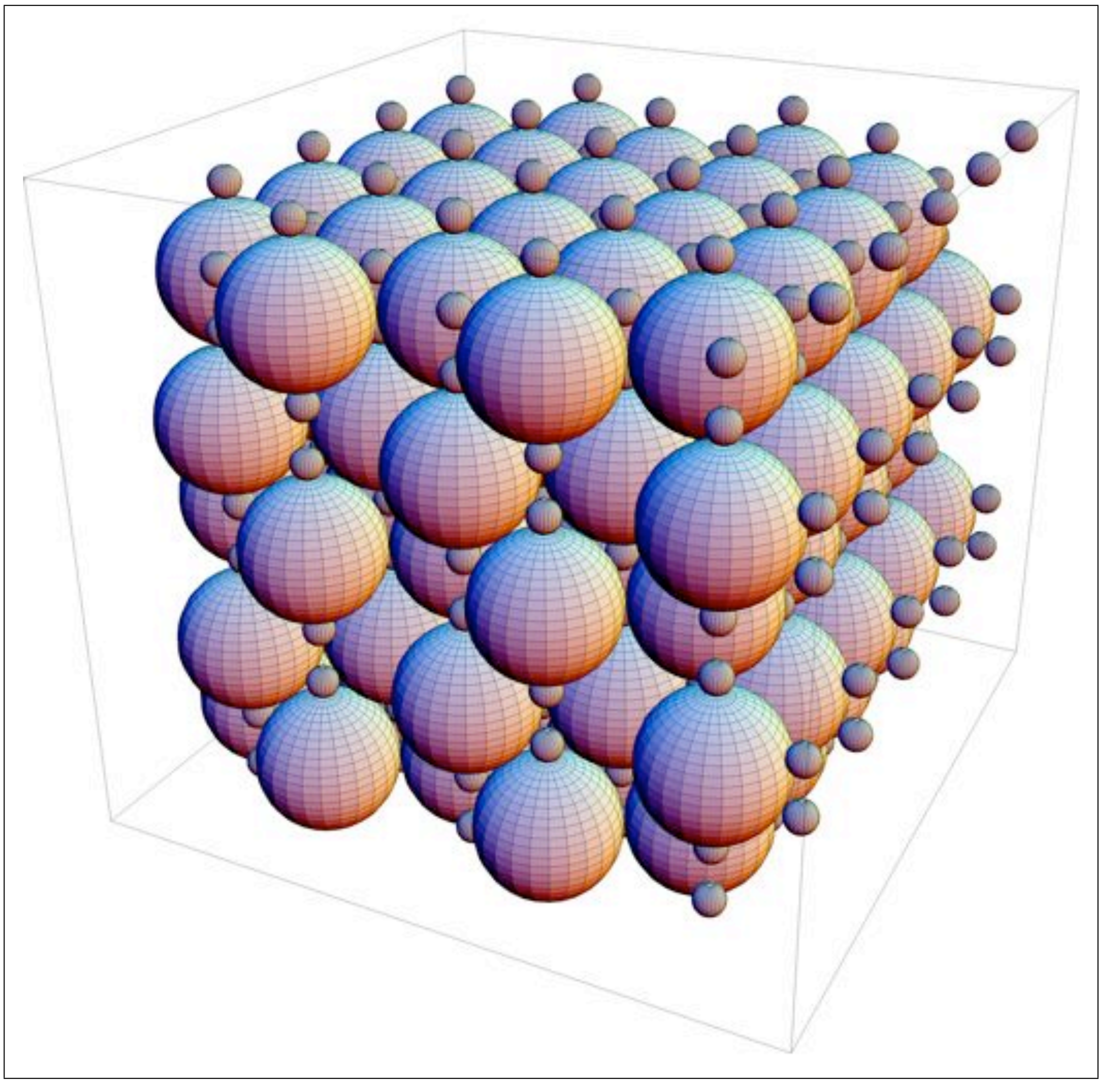

Figure 12: Smaller balls filling the voids in an already efficiently filled box.

2.5 Conclusion: The Results

Adding these smaller spheres into our lattice above increases the density from $0.740 \approx \frac{\pi}{\sqrt{18}}$ to $0.757 \approx -\frac{\pi 5\sqrt{2}}{3} + \frac{\pi 3\sqrt{3}}{2}$. The smaller spheres also help fill density lost to the sides of non-infinit boxes, this makes approaching the original $0.740 \approx \frac{\pi}{\sqrt{18}}$ quicker.

In a box 10 units on all sides, we can fill to 46.9% with just unit balls and 48.4% with the addition our smaller, void-filling balls. In a box 100 units on all sides, we can fill to 72.1% with just unit balls and 73.7% with the addition our smaller, void-filling balls.

It is generally accepted that a random, or irregular, packing of spheres comes to roughly 64% packed space. The lattice exceeds that already in some what small spaces, especially with the addition of the smaller spheres. Having a lattice also means that there is no trouble of creating a method of choosing locations of spheres as boundaries. Where in the random packing method, finding the last few open spaces for the spheres randomly is a consuming problem. This Hexagonal Close-Packed lattice is simple and provenly efficient.

2.6 Appendix: A Few More Images

When we stack balls in the real world—like on a tennis court—we generally have to put up with gravity. Here are some images that represent actual situations that could appear, gravity permitting.

Note: In Figure 13 on page 17 look for the voids that are later filled in Figure 14 on page 18. Look closer and see that there is another type of void that arises when two tetrahedron of balls meet. This void is not filled by the addition of our second lattice of balls. There is another possibility here to increase density. Another view is provided in Figure 15 on page 19, but remember that a "big" ball would normally be covering much of this different type of void.

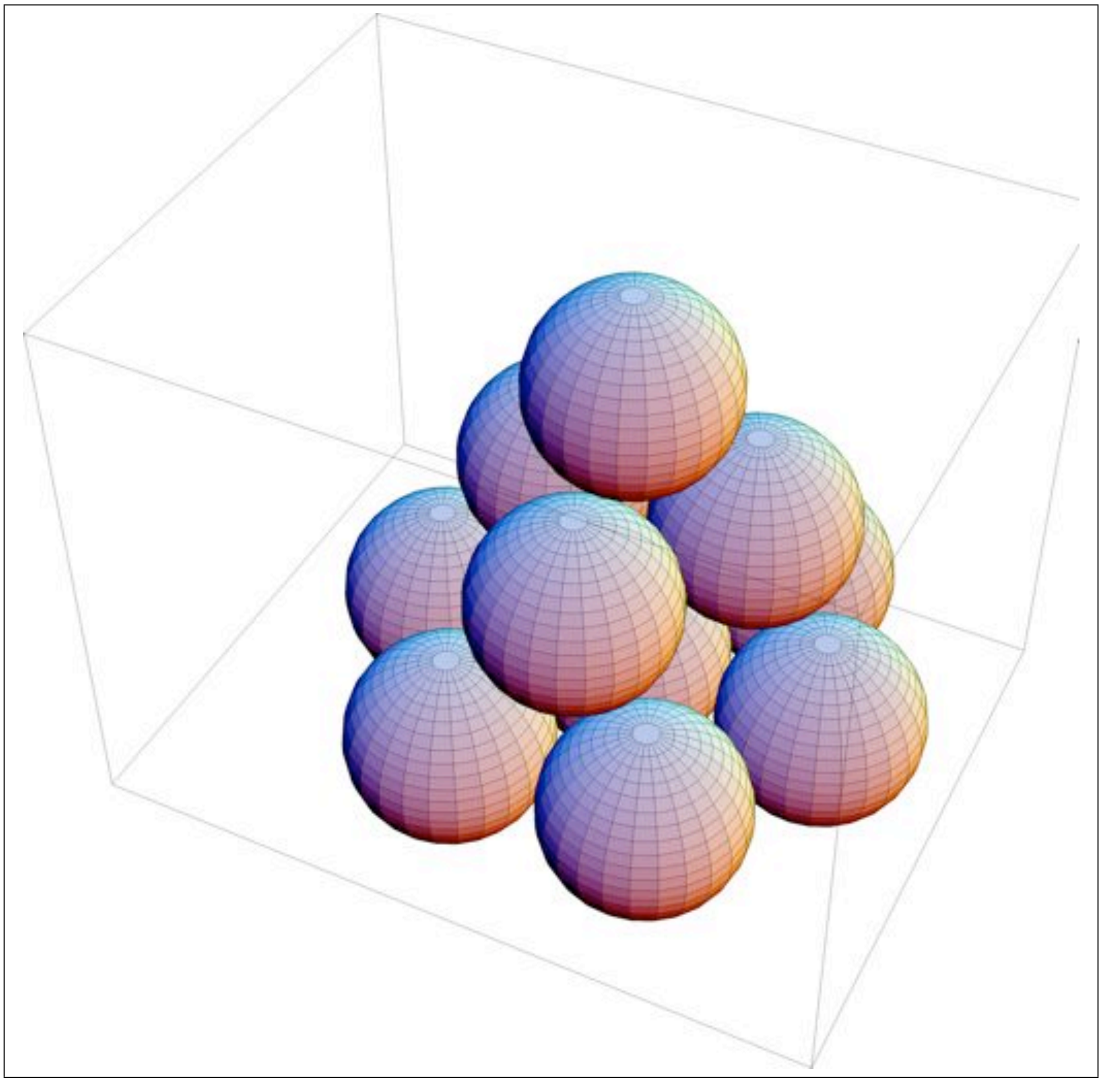

Figure 13: A "hexamid" of unit balls. There are seven balls on the base plane, then three, then one.

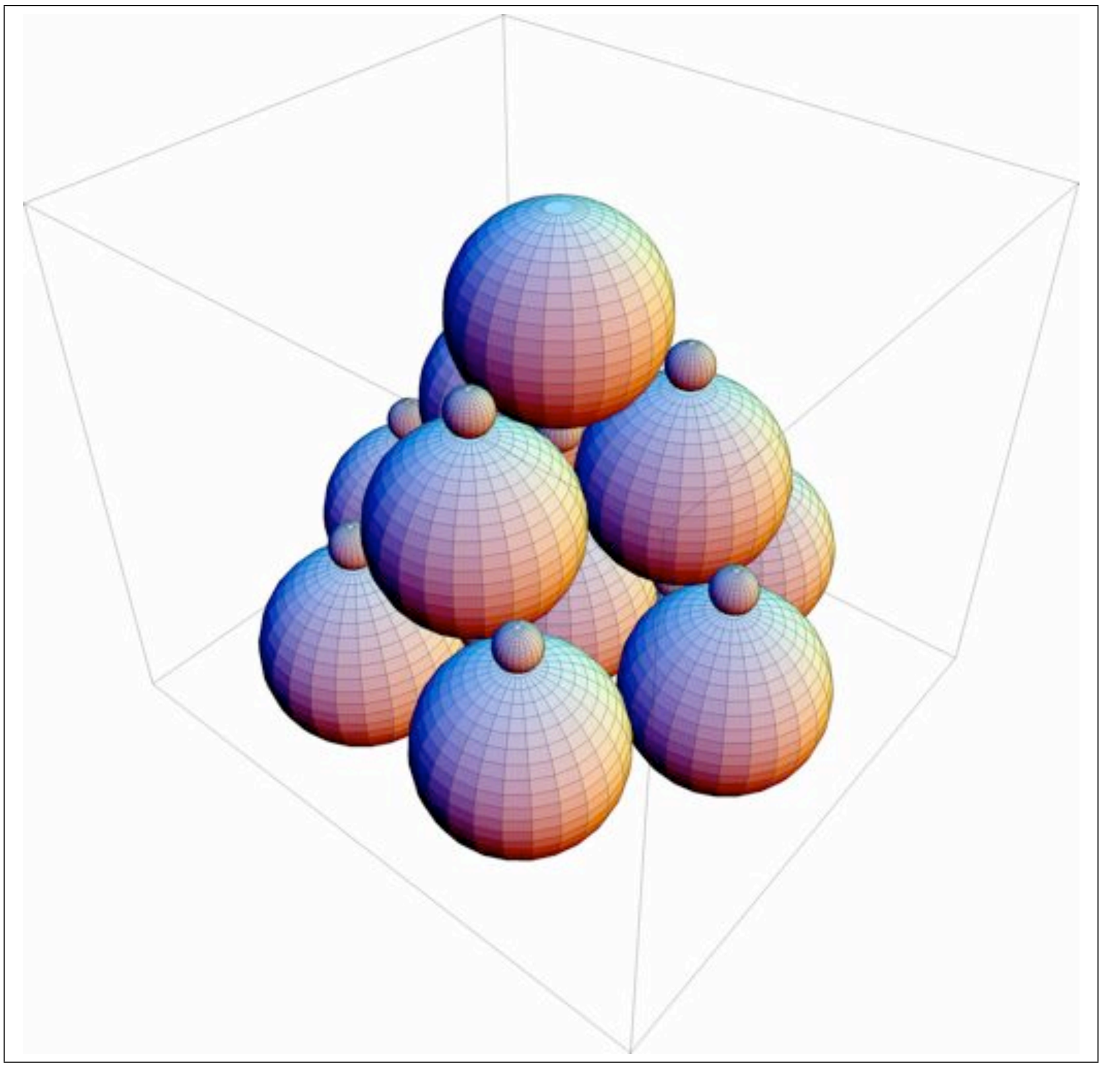

Figure 14: The same “hexamid” of unit balls, now with the addition of void-filling, smaller balls.

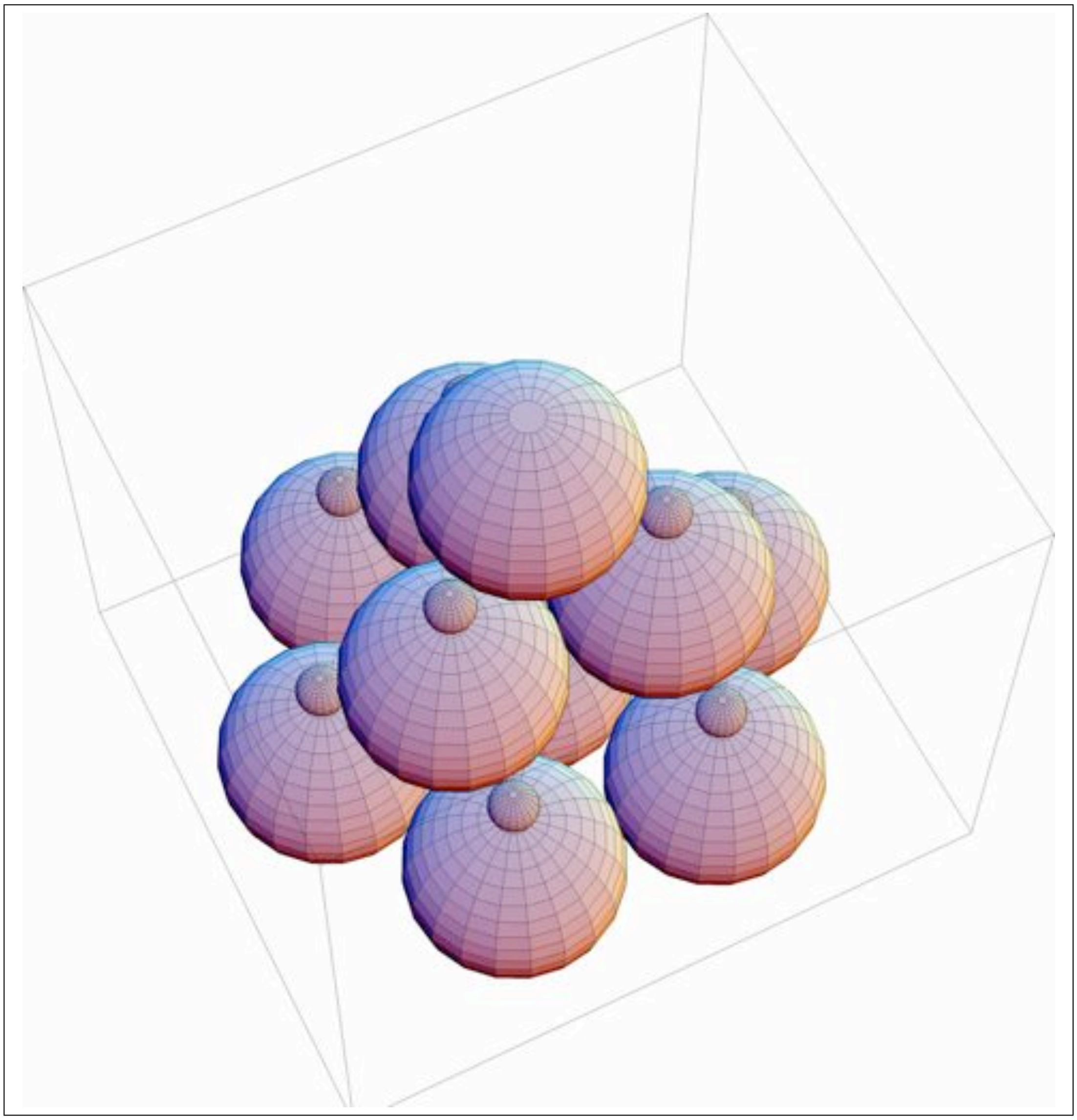

Figure 15: Another view of the “hexamid” of unit balls filled with void-filling, smaller balls.

References

[1] P. Krishna & D. Pandey, *Close-Packed Structures*, International Union of Crystallography by University College Cardiff Press. Cardiff, Wales.