Packing Uniform Spheres Within Cylindrical Constraints

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Introduction

The issue of packing uniform objects with constraints has long been a problem for merchants and industrialists looking to ship their goods. Non-tessellating objects such as spheres often have low packing efficiencies when they are randomly placed in containers. Increased packing efficiencies depend on changing the size and shape of the container based on the size and shape of the object that is being packed. Although it is difficult to prove, it is possible to arrange objects so that they optimally occupy their constrained space.

This project specifically deals with the packing of spheres in cylinders. Because of the complex nature of these packings it is very difficult to prove that one packing is more efficient than all others given the size of a container and the number of spheres. However, logical reasoning and intuition show that certain packing patterns are more efficient. All of the packings that are produced in this paper are based on the two-dimensional arrangement of equal disks in a circle. These arrangements become the three-dimensional "bases" for packing spheres in cylinders. It is the basis of this research that layering the best known two-dimensional arrangements of equal disks in a circle should result in the best known three-dimensional packings of spheres in cylinders. Optimally, one would like to produce a packing that approaches the efficiency of the densest possible packing of spheres in space, known as the Kepler Conjecture.

Johannes Kepler, better known for his mathematical descriptions of planetary motion, was the first to formally state the problem: What is the most efficient way in which spheres can be arranged in unconstrained space? He claimed that cubic close packing and hexagonal close packing (Fig. 1), which both have the same density, were the best ways to pack spheres

(Weisstein). Although the concept seems intuitively correct, no proof was produced for this claim for nearly 400 years. Only in 2003 did Thomas Hales, now at the University of Pittsburgh, produce a proof, albeit a controversial one. Hales used a computer program to execute a proof by exhaustion, eliminating all other possible packings (Hales). His proof involved over 1.2 gigabytes of code and is currently being reviewed by a panel of investigators. Some in the field believe that the use of computer programs cannot be viewed as a formal proof because they act as a substitute for the logical connections that humans use to solve such problems (Chang). Nevertheless, the mathematical community is moving forward in acknowledging Hales' proof which settles one of the oldest problems in mathematics.

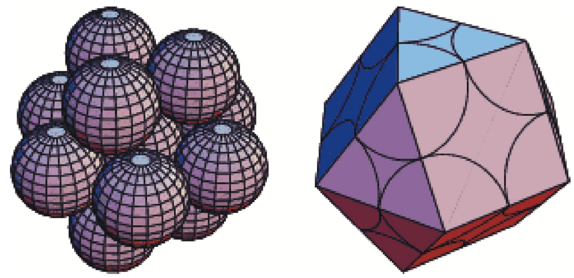


Figure 1

The Kepler efficiency, $\varphi_{Kepler} = \frac{\pi}{2\sqrt{3}} = 74.048\%$, is in reality not approachable in packing with constraints or random packings (Weisstein). Indeed, the highest efficiency obtained from close-random sphere packing is roughly 64% (Torquato). This number is still higher than efficiencies produced by many periodic packings with constraints. Generally speaking, with looser constraints (or a larger container as compared to the size of the particle), a higher packing efficiency can be obtained. This is because particles in the center of the container have a much greater opportunity to come into contact with other particles, as opposed to those adjacent to the boundaries (Smith et al.). This is extremely important for an efficient packing because more contacts are the equivalent of a higher efficiency. The maximum number of contacts that any one sphere can have with surrounding spheres of equal size is twelve, which is exhibited by the spheres in hexagonal-close packing (Weisstein).

To optimize the packing of spheres in a cylinder, initial considerations include what the proper dimensions of the container should be for the size and number of spheres to be packed. There are, of course, an infinite number of right cylinders that can be created but not all of them deserve consideration. The ones that can be used to form dense, periodic packings are those which are worth investigating, and in all likelihood these are ones in which the base fits an integer number of spheres in the most compact way possible. This is the equivalent of packing two-dimensional disks in a circumcircle, and this is how the exact dimensions of the bases of the cylinders used for this project were chosen. The two-dimensional packings were based on the results of many years of geometrical investigations by mathematicians. The packings of one, two, three, and four equal circles (fig. 2) within a larger circle are each considered to be self-evident that they are indeed the optimal packings (Kravitz). Optimal packings from 5 to 11 disks in a circle have each been proved. No packing of 12 or more circles have been proved to be the most efficient. In recent years computer algorithms have been used to find tight two-dimensional packings of up to 65 disks in a circle (Graham et al.). It is unlikely that any of these packings involving such high numbers of particles will ever be proved optimal because such a proof would be extremely complex, tedious, and inconsequential.

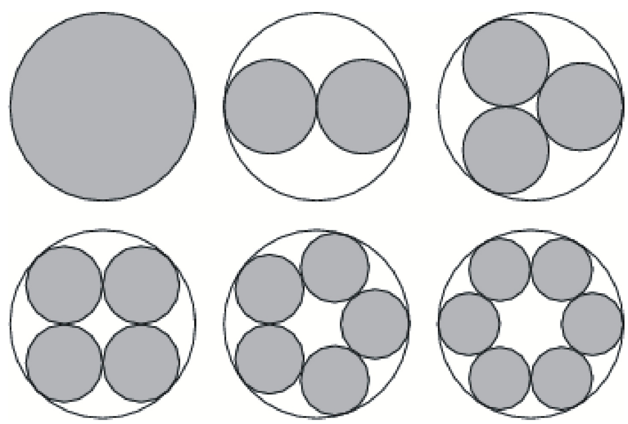


Figure 2

Despite the fact that many two-dimensional packings cannot be proved to be the most efficient, intuitive reasoning shows that many of them are superior to all other known packings. This is most evident in the curved hexagonal packing series $h(k) = 3k(k + 1) + 1$ (Fig. 3), for hexagonal number h, where the circles align themselves with one of six curved arms extending from the center (Lubachevsky and Graham). These packings mimic the most efficient packing of circles in a plane which is in the form of a basic honeycomb pattern.

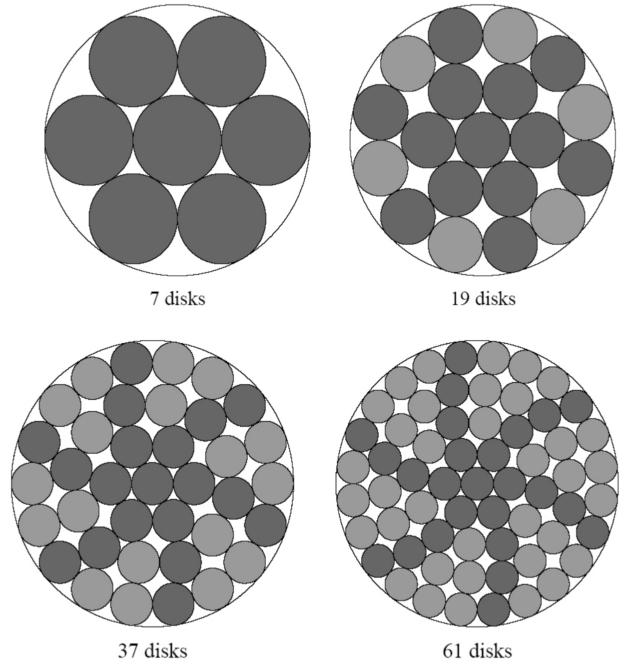


Figure 3

Hypothesis

The central hypothesis of this paper is that the stacking of the most efficient arrangement of two-dimensional disks in a plane will result in the most efficient known packing of three-dimensional spheres in a cylinder. A glance at the most efficient known base layers intuitively shows that this is a reasonable assumption for most, if not all, of the packings. This does not exclude the possibility of more efficient three-dimensional packings being found, but it does suggest that it would involve a revised, more efficient base-layer as well. In addition to the central hypothesis, three additional sub-hypotheses are added to address the different methods of investigation of the central hypothesis.

Base-Layers 1 - 5: Due to the simplicity of these packings (see fig. 2) and their invariance under a rotation of $\frac{2\pi}{n}$ radians, repeated stackings of these layers should result in a limit in efficiency with an infinite number of layers. In addition, it may be possible to develop a proof for some of these packings to establish them as the most efficient packing of spheres within a cylinder.

Base-Layers 3*k*(*k* + 1) + 1: This series of curved hexagonal packings appears as though it would stack in layers that are mathematically easy to represent. A limit of efficiency with infinite levels in also sought here, although the methods used would not be the same as that of the previous section. It is important to note that the base-layers $3k(k + 1)$ and $3k(k + 1) + 1$ result in equal packing configurations and, therefore, only base-layers $3k(k + 1) + 1$ were investigated.

Base-Layers 8 - 17: Mathematical analysis of these layers may prove to be exceedingly complicated but physical experimentation will be used in its place to show that the most efficient packings are indeed the layering of the most efficient base layers.

Methods

Base Layers 1-5:

The first five two-dimensional arrangements of disks in a circle are very straightforward and did not require computer simulation or experimental testing to show the manner in which these three dimensional bases should be layered. The efficiency of the packings of bases 1-5 are all easily described by the ratio φ of the volume of the spheres with radius 1 (r = 1) V_s, divided by the volume of the cylinder, V_c :

$$\varphi = \frac{V_s}{V_c} = \frac{NL\left(\frac{4}{3}\pi r^2\right)}{\pi R^2 (H(L-1)+2)} = \frac{4NL}{3R^2(H(L-1)+2)}$$ **Equation 1**

where N is the number of spheres per level, L is the number of levels, R is the radius of the encompassing circle, and H is the additional height per level. A table of H and R values for the first 5 bases follows.

Table 1

N	1	2	3	4	5
R (in radii)	1	2	$1+\frac{2\sqrt{3}}{3}$	$1+\sqrt{2}$	$1+\sec\left(\frac{3\pi}{10}\right)$
H (in radii)	2	$\sqrt{2}$	$\sqrt{\frac{8}{3}}$	$\sqrt{2\sqrt{2}}$	$\sec\left(\frac{3\pi}{10}\right)$

Base Layers 3*k*(*k* + 1) + 1:

When arranged in curved hexagonal packings, bases 7, 19, 37, 61, and 91 (k = 1, 2, 3, 4, 5 respectively) have very high efficiencies because they form extremely “tight” packings (Graham et al.). The efficiencies of these packings are especially high in two dimensions, so one would expect that layering “tight” levels of spheres would result in very efficient three-dimensional packings. However, it is difficult to qualify this statement using Equation 1 because the packing is not cyclic. When layering $3k(k + 1) + 1$ bases on top of one another, the outer rings of spheres lie in the gaps left by the preceding layer under a rotation of $\pi/6$ radians. The sphere in the center of the packing is forced to rest directly on top of the center sphere of level directly below it, thus producing a greater height in the center than in the outer rings.

To accurately simulate the efficiency of such a packing, a computer application was developed to calculate the height of the packing for each sphere added and then calculate an efficiency. The code was written in Basic and instructed the program to add $3k(k + 1)$ spheres to the outer rings for every 1 sphere added to the center. The program took into account the fact that for every center sphere added the height was increased by two radii, and adding a full ring of spheres raised the height $\sqrt{3}$ radii. When the difference between the inner height and the outer height became greater than two radii, the program added an additional layer to the outer rings and then reverted to former calculations (Fig.4). The height values produced by the computer were inserted into an Excel spreadsheet where they were calculated into efficiencies. The investigations of the $3k(k + 1) + 1$ series end with $k = 5$ because $k = 6$, 7, and 8 do not produce curved hexagonal packings that are more efficient than other known two-dimensional packings involving equal numbers of disks.

Base Layers 8-17:

Each of the most efficient two-dimensional bases of 8-17 disks are either unsymmetrical or do not allow for contact between adjacent disks in the outer ring. It is extremely difficult to express mathematically how the layering of such packings would develop because each additional layer becomes more distorted from its original shape than the preceding layer. In the cases where all disks in the outer ring remain in contact with their two adjacent disks (8, 9, 11, 13) it is easy to calculate the height of the outer ring and thus find an approximation for the overall height of the packing. However, the interior spheres do not layer with any regularity so it remains difficult to determine a limit in efficiency.

To investigate the packings of bases 8 through 17, physical experiments were devised to produce random packings of spheres within the cylindrical constraints. A precise definition of random packing has only been developed for spheres packed in infinite space. For the purposes of this experiment, random packing was defined as ball bearings placed simultaneously into a cylinder with gravity as the sole force that determines the final placement of the bearings. The stainless steel ball bearings have a radius of 4 millimeters with a diametric tolerance of +/- 25 microns. The cylinders were created using a lathe that bore holes in inch-thick (25.4 mm) cross sections of a polycarbonate cylinder accurate to a thousandth of an inch (0.0254 mm). The radii of holes were deliberately made two-thousandths of an inch (.0508 mm) larger than the smallest diameter allowed by the two-dimensional close packings. This allowed for the bearings to be tightly packed but not jammed when occupying a single level of the cylinder (Fig. 6).

A shake table was designed to ensure that all the particles were in an equally random state before gravity took effect. Two 1'×1' pieces of single-ply balsa formed the top and bottom of the table. Four springs were attached to each of the four corners of the balsa sheets. A 3-volt motor with a five gram mass affixed to its axle was secured to one side of the top of the table. The two 1.5-volt AA batteries that power the motor were placed in brackets and secured to the opposite side of the table, which helped to distribute the weight evenly to all springs. Four clips were attached to the center of the table to hold the cylinder in place. A potentiometer and switch were attached to the bottom of the table to control the motor. When turned on, the mass at the end of the axle rotated to produce a torque which caused strong oscillations. The potentiometer was set to apply to 2.5 volts to the motor, which produced strong oscillations with an amplitude of roughly one millimeter. These parameters were held constant throughout experimentation (Fig. 5, 7, 8).

Experimental procedure begins with the motor turned on so that the spheres enter the cylinder with maximum oscillations of the shake table. A funnel is used to pour the ball bearings into the cylinder and they are shaken for five seconds after the funnel is removed. The amount of time the bearings are shaken does not effect their final packing. The oscillations are constant while the motor is on so the positions of the bearings are equally random at all times. Five seconds is thus an arbitrary parameter used to maintain consistency throughout the experiment. Once the motor is turned off the oscillations stop and the balls settle into place. Calipers were used to determine the height of the ball that settled in the highest position. This height was taken as the height of the cylinder which in turn was used to calculate the efficiency of the packing. Two separate experiments were designed. One focused solely on base-layer 8 while the other investigated base-layers 9-17. For base-layer 8, ten trials were conducted for every bearing added. For base-layers 9-17, ten trials were conducted for every base, with six layers of balls packed.

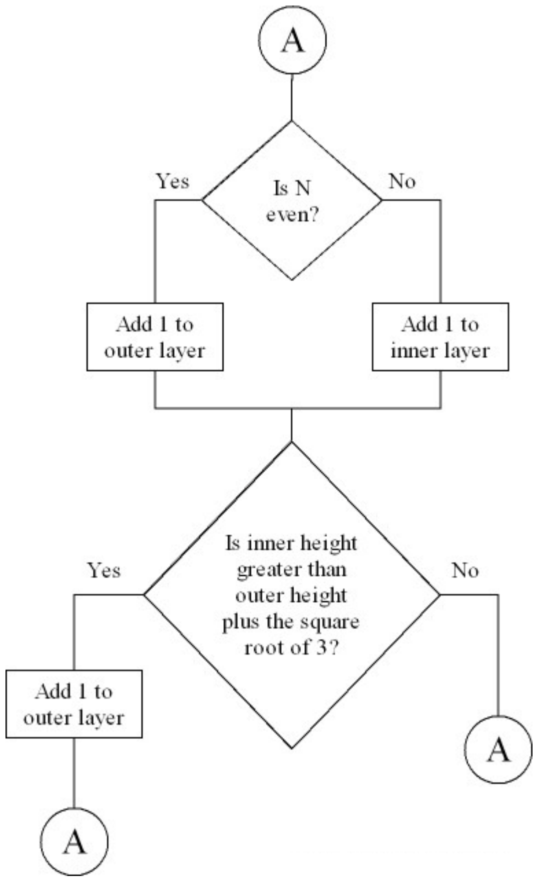


Figure 4

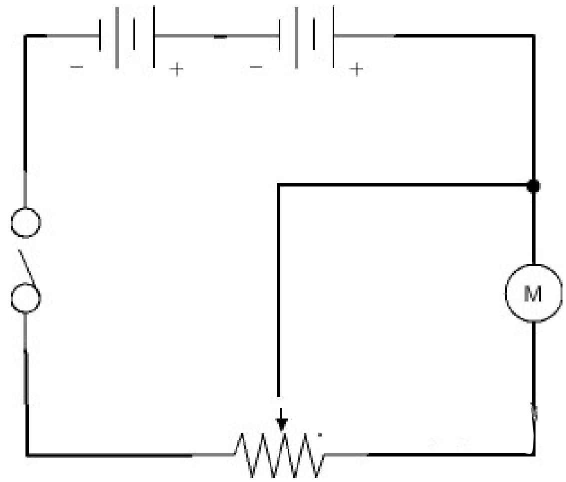
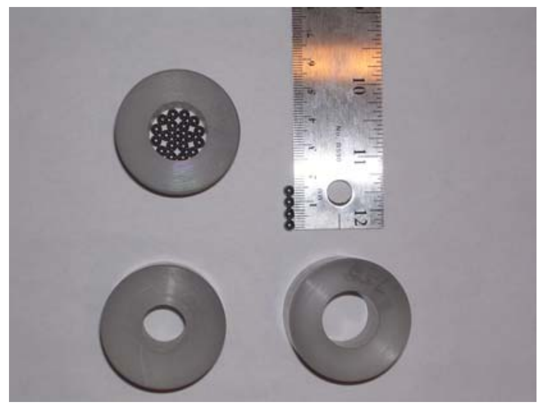


Figure 5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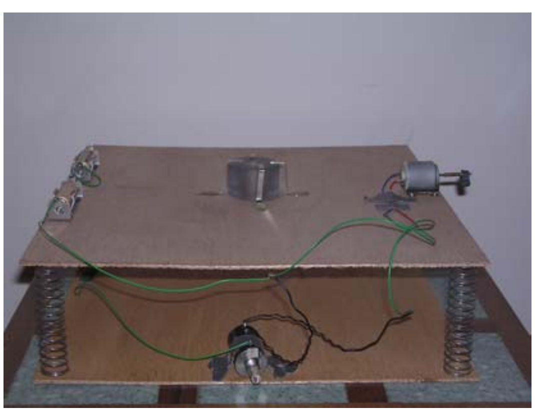


Figure 7

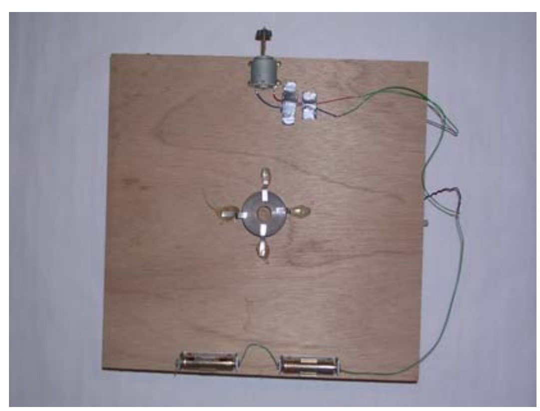


Figure 8

Results and Discussion

Base Layers 1-5:

The efficiencies of the first five base-layer packings increased asymptotically with additional layers as seen in Graph 1. Equation 2 was derived by applying L'Hôpital's Rule to Equation 1 to find the limit of efficiency with infinite levels. The limits at infinity of bases 1 through 5 are listed in Table 2.

$$\lim_{L\to\infty}\left(\frac{4NL}{3R^2\left(H(L-1)+2\right)}\right)=\frac{4N}{3R^2H}$$ **Equation 2**

Table 2

N	1	2	3	4	5
φ	.6666666667	.4714045208	.527596353	.5440951573	.5370086351

The calculated efficiencies represent the best packing of spheres in a cylinder of the given radius and infinite height. Each of these five base-layers have been proven to be the most efficient possible packings in two dimensions. In three dimensions, each layer is rotated π/N radians so that the spheres rest in the lowest possible positions created by the previous layer. The fact that both the base configuration and layering height can be proved to be most efficient is strong evidence that these packings are the most efficient possible. However, a formal proof must exclude the possibility of any other more efficient packing and there are great difficulties in creating such a proof.

Base Layers 3*k*(*k* + 1) + 1:

The results from the Basic application are displayed in Graphs 2 and 3. When only a small range of data is sampled, the irregularities of the graph are very apparent. The kinks appear as the computer program compensates for the height differential between the inner and outer layers, adding an outer layer when necessary. However, when a much larger data range is sampled, the graphs appear similar to those produced for base-layers 1 through 5. This confirms the existence of a limit at infinity of this semi-cyclic packing. However, a purely mathematical approach was needed to determine the precise value of the limit.

Take for example $k = 1$, which is base-layer 7. Let s represent the number of layers in the center column and r represent the number of layers in the outer ring. The height of the interior column is therefore $2s$ because each sphere lies directly on top of the one below it. In the outer ring the height is $r\sqrt{4-\left(\csc\left(\frac{5\pi}{12}\right)\right)^2}+2$. To simplify the efficiency equation, the outer height will simply be considered $r\sqrt{3}$ because the height of the outer ring in the $3k(k + 1) + 1$ series is

$$h=\sqrt{4-\left(\csc\left(\frac{(6k-1)\pi}{12k}\right)\right)^2}$$ **Equation 3**

which rapidly approaches $\sqrt{3}$ with higher values of k. The overall height of the cylinder is the maximum of these two values for a given r and s. This mathematical description is also considerate of the physical properties of the packing, so there can never be a difference of more than $\sqrt{3}$ between the inner and outer height, for this would create an unstable situation. Since we are considering a limit at infinity, the additional 2 radii in the outer layer need not be considered. In addition, the height can be either 2*s* or $r\sqrt{3}$ because the maximum difference between the heights is insignificant with infinite layers. Therefore:

$$2s \approx r\sqrt{3} \rightarrow \frac{2}{\sqrt{3}} \approx \frac{r}{s}$$

$$\frac{4N}{3R^2H} = \frac{4(6r+s)}{3(3)^2(2s)} = \frac{12r}{27s} + \frac{2}{27} = \frac{12(2)}{27\sqrt{3}} + \frac{2}{27} = .587$$ **Equation 4**

In this equation the total number of balls packed was represented by $6r + s$ because there were six balls in the outer ring and one in the middle. The height was taken as 2*s* because the actual height must be within $\sqrt{3}$ of this number. This is a close approximation as *r* and *s* tend proportionately towards infinity although there is an error term described by the Equation 4. The term goes to zero as the height goes to infinity. It is possible to determine a limit of all packings with base layers $3k(k + 1) + 1$. This limit describes the densest packing of spheres when configured in curved hexagonal formations in each layer. First note that:

$$\varphi(k) = \frac{4(3k(k+1)r+s)}{6\left(1+\csc\left(\frac{\pi}{6k}\right)\right)^2 s} = \frac{4\left(k^2+k\right)\sin^2\left(\frac{\pi}{6k}\right)}{\sqrt{3}\left(\sin\left(\frac{\pi}{6k}\right)+1\right)^2} + \frac{2}{3\left(\csc\left(\frac{\pi}{6k}\right)+1\right)^2}$$

and compute the limit as follows:

$$\lim_{k\to\infty}\left(\varphi(k)\right)=\frac{\lim_{k\to\infty}\left(4\left(k^2+k\right)\sin^2\left(\frac{\pi}{6k}\right)\right)}{\lim_{k\to\infty}\left(\sqrt{3}\left(\sin\left(\frac{\pi}{6k}\right)+1\right)^2\right)}+\lim_{k\to\infty}\left(\frac{2}{3\left(\csc\left(\frac{\pi}{6k}\right)+1\right)^2}\right)$$

$$=\frac{\lim_{k\to\infty}\left(4\left(k^2+k\right)\sin^2\left(\frac{\pi}{6k}\right)\right)}{\sqrt{3}}$$

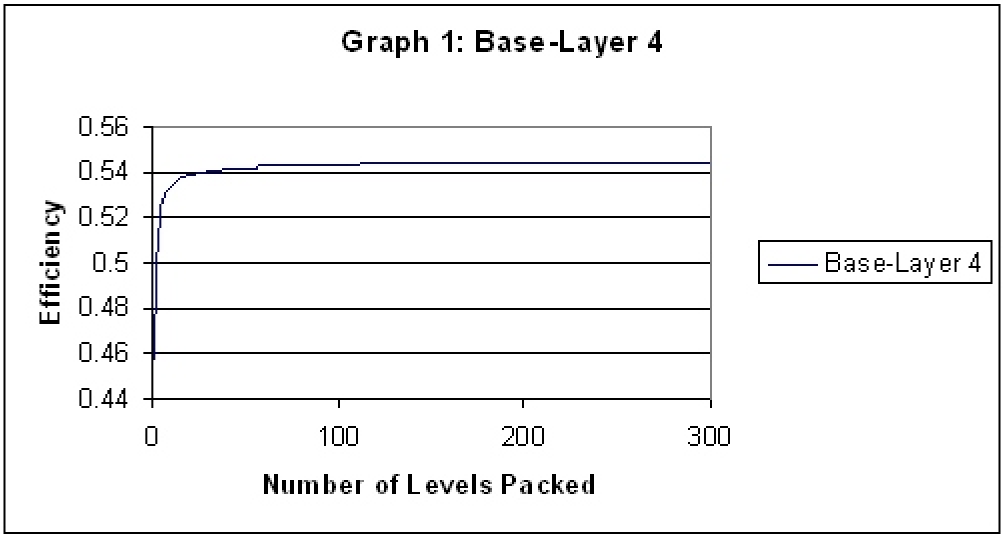
Then make the change of variable $k=\frac{1}{t}$ so:

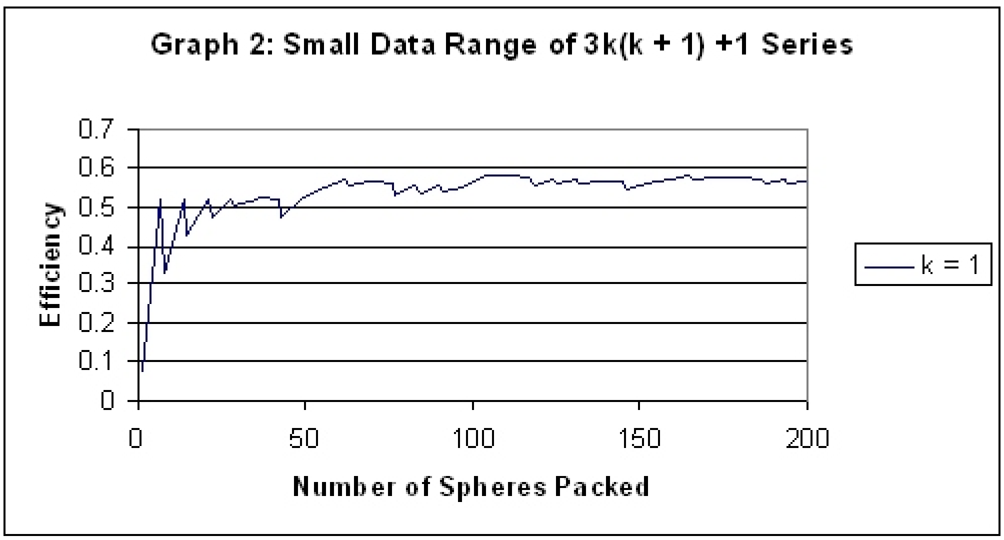
$$\lim_{k\to\infty}\left(\varphi(k)\right)=\lim_{t\to 0+}\left(4\left(\frac{1}{t^2}+\frac{1}{t}\right)\sin^2\left(\frac{\pi t}{6}\right)\right)=\lim_{t\to 0+}\frac{4\sin^2\left(\frac{\pi t}{6}\right)\left(\frac{\pi^2}{36}\right)}{t^2\left(\frac{\pi^2}{36}\right)}=\frac{\pi^2}{9}$$

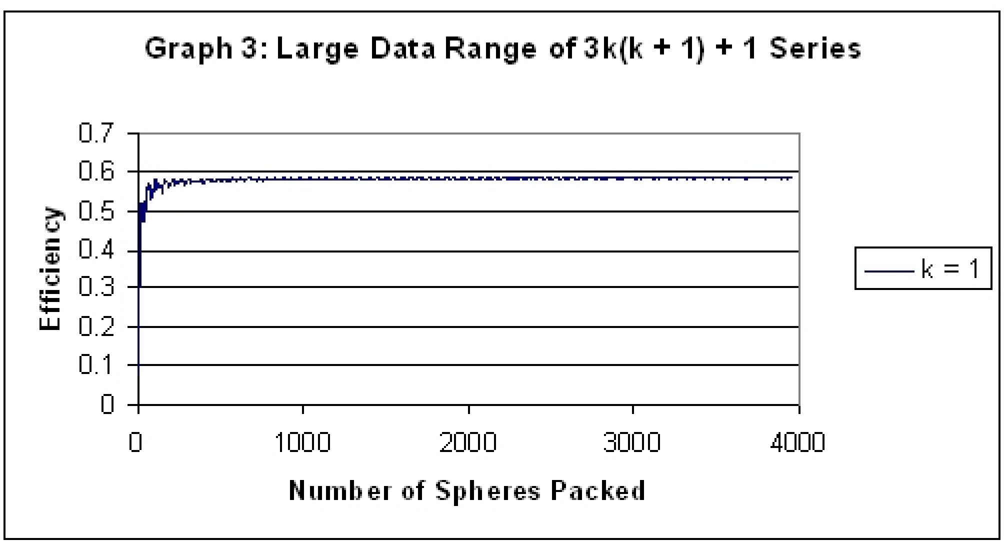
$$=\left(\frac{\pi^2}{9}\right)\left(\frac{1}{\sqrt{3}}\right)=\frac{\pi^2\sqrt{3}}{27}\approx 0.6331354175$$

Equation 5

The first step in the equation packs a total of $3k(k+1)$ spheres into the outer rings and a single sphere in the center column for every layer of *r* and *s* respectively. The formula for the radius was derived by Lubachevsky and Graham in their paper on curved hexagonal packings in a plane (Lubachevsky and Graham). The final value of the expression yielded an efficiency over 10 percent less than that of the Kepler conjecture. This is not surprising, considering the fact that the equivalent packing of curved hexagonal disks in two dimensions is nearly 10 percent less than


Graph 1: Base-Layer 4
Efficiency
0.56
0.54
0.52
0.5
0.48
0.46
0.44
0
100
200
300
Number of Levels Packed
Base-Layer 4


Graph 2: Small Data Range of 3k(k + 1) +1 Series
Efficiency
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
50
100
150
200
Number of Spheres Packed
k = 1


Graph 3: Large Data Range of 3k(k + 1) + 1 Series
Efficiency
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
1000
2000
3000
4000
Number of Spheres Packed
k = 1

that of the optimal hexagonal packing of circles in a plane (Lubachevsky and Graham). In addition, certain higher values of *k* do not yield dense packings in two dimensions. For values of *k* = 6, 7, and 8, better packings can be formed by not using curved hexagonal configurations, yet *k* = 9 yields a packing of disks better than other known packings.

Base Layers 8-17:

The data collected from the trials for base-layers 9-17 represents the average of the ten trials in which the final height was recorded after shaking six base-layers worth of ball bearings. The data from these trials were compared to the values found by layering the base-layers by hand in an ordered fashion. In no instance did the efficiency of the randomly packed ball bearings exceed that of the bearings placed by hand. Data Table 3 compares the experimental values with the hand-packed values and also gives a standard deviation for the experimental data. It is important to recognize that both values were experimentally found. Although in some cases the standard deviation allows for the packing efficiencies to be in range of the calculated efficiencies, at no point in experimentation did that actually occur. While this does not prove that the packings based on precise layering of spheres are the most efficient possible, it does suggest that method of base-layering would produce the most efficient possible base layering.

A more thorough investigation was undertaken for base-layer 8. Base-layer 8 was chosen for several reasons. It is a simple configuration with 7 disks packed in the outer ring with one “rattler” (Fig. 9) It resembles other well explored packings like base-layer 7 and this packing has been proven to be the most efficient in two dimensions. It is easy to calculate the height of the outer ring as the spheres are layered under a rotation of radians, but it

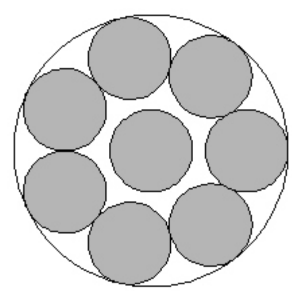


Figure 9

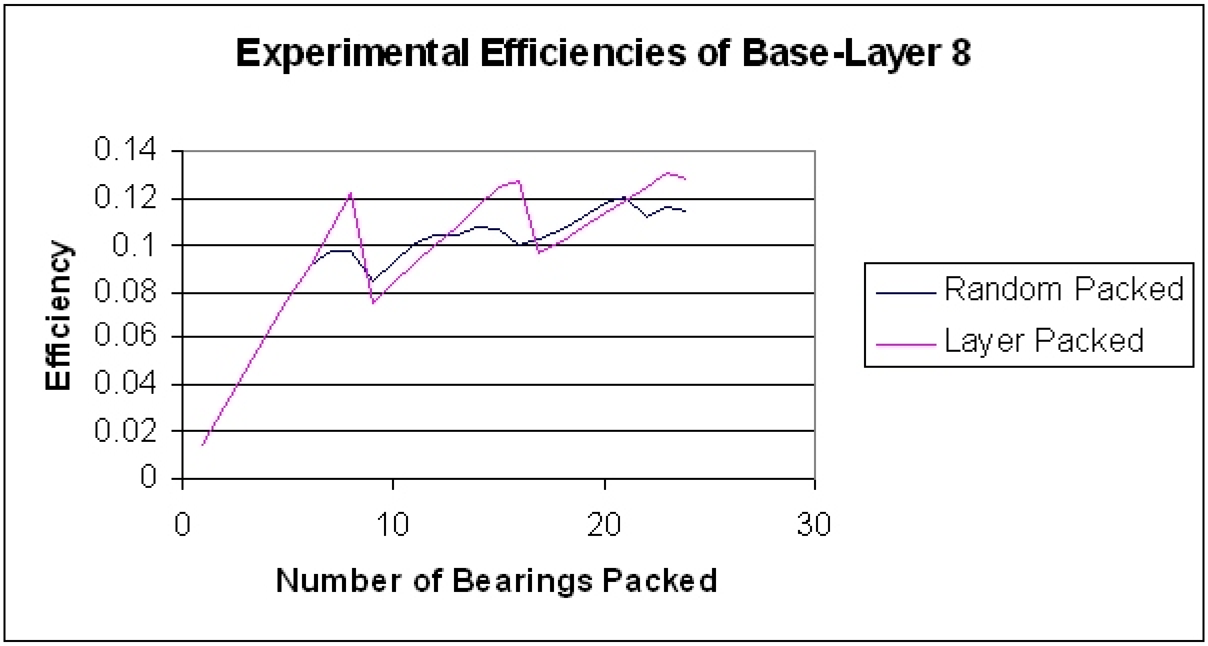
becomes very difficult to predict the placement of the inner spheres after just two stacked layers.

This packing was investigated on a sphere by sphere basis and ten trials were made for each value of n up to 25. A standard deviation was also found for each set of trials and these were compiled to make Graph 4. In many ways the graph mimics that of base-layer 7. The graph is relatively continuous over intervals that would normally be of a single level, and the graph jumps at intervals when an additional layer would have been added. Yet there were only a select few trials in which the random packing allowed the balls to settle into the hand packed configuration. When the two graphs are compared it appears that the experimental graph has simply been shifted over by one particle along the x-axis, as though it were packing an additional ball bearing per trial.

Table 3

Base-Layer	Hand-Packed φ	Random φ	Standard Deviation
9	0.5168	0.4986	0.0154
10	0.5213	0.5064	0.0272
11	0.5389	0.5238	0.0243
12	0.5813	0.5432	0.0457
13	0.5408	0.5318	0.0272
14	0.5381	0.5309	0.0262
15	0.5334	0.5273	0.0258
16	0.5604	0.5367	0.0272
17	0.5481	0.5245	0.0297

Graph 4



Conclusion

The results of the mathematical analysis of the ordered packings support the hypothesis that the most efficient known two dimensional base-level configurations yield the most efficient three dimensional packings. The limits of the packings of base-layers 1 - 5 are not only highly ordered, but they occupy the space in the most logically reasonable patterns. Although the calculated packings of the base-layers 8-17 surpassed the obtained experimental values, there is little evidence that these are the most efficient packings given the degenerate nature of their layerings. The limit of the $3k(k + 1) + 1$ series of packings far exceeded all other packing efficiencies found during mathematical and physical experimentation. However, the fact that these efficiencies are less than the Kepler efficiency shows that cylindrical packing is not optimal when large numbers of particles are to be packed.

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