Investigating Cross-Sectional Size Distribution of Randomly Distributed 3D Spheres

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***Abstract*—Text Text**

I. Introduction

In the world of Material Science and Crystallography, it is often the case that a material is identified and classified using the distribution of its constituent particle sizes. However, direct observation of the particles so as to construct a distribution is often impossible. Using a modern microscope or laser imaging techniques, it is possible to observe particles in a cross-section of material. But the observed radii of particles in this cross-section do not necessarily correspond directly to the radii of the particles in the material, since the plane of the cross-section is not necessarily oriented such that the observed particles lie exactly on the plane. Thus, it becomes difficult to relate the observed distribution of particle sizes in the plane to the real distribution of particle sizes in the material.

Mathematically, determining the distribution of spherical particles from planar sections is a well known problem called
cite Wicksell's Corpuscle Problem , named after S. D. Wicksell, who solved the problem in 1925. With this solution, it is possible to determine the original distribution of spherical particles. Thus, it is possible to determmine the distribution of particle sizes in a solid from its observed cross-section,
nasa allowing us to identify and classify materials better .

In this paper we aim to show that it is possible to reproduce theoretical results on cross-sectional distributions using numerical simulation, and it is thus possible to solve Wicksell's Corpuscle Problem in this manner.

II. Method

Consider many spheres of different radii distributed randomly in space. For the purposes of the numerical simulation, we will consider a cube of length 20. The spheres were not allowed to overlap, which we ensured by placing the spheres such that if one sphere has vector position $\overrightarrow{\mathbf{a}}$ and radius r_1 and the other has vector position $\overrightarrow{\mathbf{b}}$ and radius r_2, the spheres must have positions such that:

$$|\overrightarrow{\mathbf{a}} - \overrightarrow{\mathbf{b}}| > (r_1 + r_2)$$

Random coordinates for a sphere are drawn from a uniform distribution and checked against every existing sphere until a set of coordinates is drawn that ensures no overlap, at which point the sphere is placed in space and the process is repeated until all the necessary spheres have been placed.

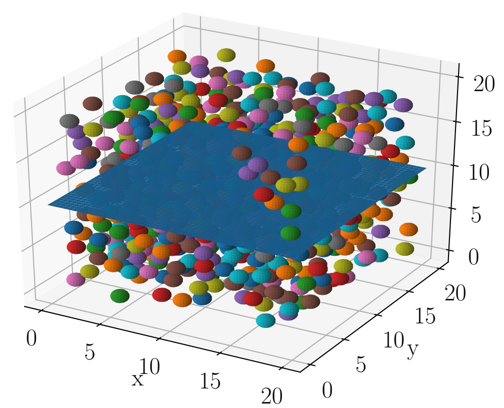


Fig. 1. 750 spheres of radius 0.7 distributed randomly in a cube of length 20, such that no sphere is touching or overlapping another sphere. A randomly oriented plane passes through the box and "cuts" through the spheres.

We then placed a plane into the cube, with a random orientation. The plane will "cut" through many of the spheres in the cube. This is shown in Figure 1. Here we see 750 spheres, each with radius 0.7 distributed randomly in a cube of length 20. The plane is shown in blue, and can be seen intersecting many of the spheres in the cube.

In order to obtain the planar cross-section, we employed the spherical cap method . If we consider a sphere with centre cite
$\overrightarrow{\mathbf{c}_0} = (x_0, y_0, z_0)$ and radius R, and a plane with equation $Ax + By + Cz = D$ such that $\overrightarrow{\mathbf{n}} = (A, B, C)$ is the normal vector to the plane, then the distance from the centre of the circle to the closest point on the plane p_0 is given by ρ:

$$\rho = \frac{(\overrightarrow{\mathbf{c}_0} - \overrightarrow{\mathbf{p}_0}) \cdot \overrightarrow{\mathbf{n}}}{|\overrightarrow{\mathbf{n}}|} = \frac{Ax_0 + By_0 + Cz_0 - D}{\sqrt{A^2 + B^2 + C^2}}$$

If $|\rho| < R$, then there is an intersection of the plane and the sphere. The radius of the circle r in the planar cross-section is given by:

$$r = \sqrt{R^2 - \rho^2}$$

And we then binned this radius to produce a histogram of the distribution of planar circle radii. It is also possible to recover the centre $\vec{\mathbf{c}}$ of the circle visible on the plane using:

$$\vec{\mathbf{c}} = \vec{\mathbf{c}_0} + \rho \frac{\vec{\mathbf{n}}}{|\vec{\mathbf{c}}|} = (x_0, y_0, z_0) + \rho \frac{(A, B, C)}{\sqrt{A^2 + B^2 + C^2}}$$

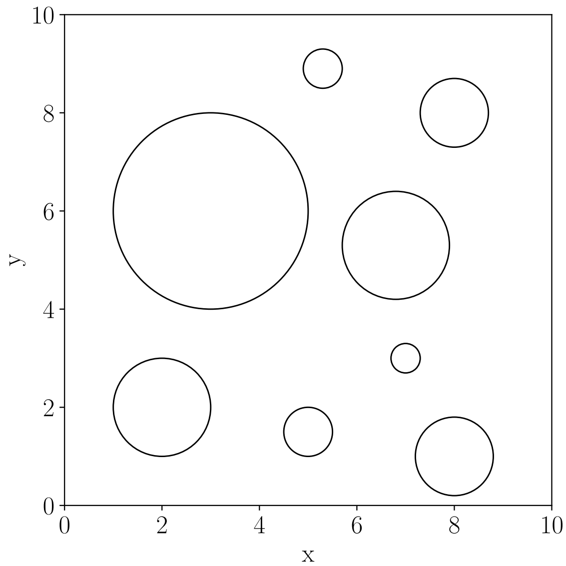


Fig. 2. Planar cross-section constructed using mock data. Spheres cut by the plane appear as circles on the plane, with radius dependent on the relative position of the spheres to the plane. This distribution of circles can be modelled.

Figure 2 presents a planar cross-section generated using this method and mock data. As we see, there are a range of circular radii observed since even though the spheres all had the same radius, they were at different distances from the plane, and were thus cut at different points. The many observed circular radii are binned to produce a distribution.

If $f(R)dR$ is the number of spheres per unit volume with radii in interval $[R, R+dR]$, then we can define a distribution $\phi(x)dx$ which represents the number of circles per unit area on the plane with radii in interval $[x, x+dx]$. This distribution is given by:

$$\phi(x) = \int_x^\infty \frac{x f(R)}{\sqrt{R^2 - x^2}} \tag{1}$$

We can compute this integral to obtain a theoretical planar distribution for different starting spherical radius distributions.

We first considered the case in which all the spheres had the same radius R_0. In this case, the spherical radius distribution is simply a Dirac delta function centred on the radius R_0.

If we compute the integral in Equation 1, replacing $f(R)$ with $\delta(R - R_0)$ we find:

$$\phi(x) = \int_x^\infty \frac{x\delta(R - R_0)}{\sqrt{R^2 - x^2}} = \frac{xH(R_0 - x)}{\sqrt{R_0^2 - x^2}} \tag{2}$$

where $H(R_0 - x)$ is the heaviside function, which "turns on" the distribution only for $x < R0$ as it is not possible to have a circular radius x larger than the spherical radius. So we aim to see our experimental data reproduce this distribution. We also investigated how changing the value of R_0 affects the experimental distribution.

We next considered the case in which each sphere has a radius R uniformly distributed in a range $R_1 < R < R_2$. In this case, we modify $f(R)$ in Equation 1 to be:

$$f(R) = \begin{cases} 1, & \text{if } R_1 < R < R_2 \\ 0, & Otherwise \end{cases}$$

In this case the integral in Equation 1 does not need to be computed with the limits shown, but instead with limits between R_1 and R_2 since $f(R)$ is 0 otherwise:

$$\begin{aligned} \phi(x) &= \int_{R_1}^{R_2} \frac{x f(R)}{\sqrt{R^2 - x^2}} \\ &= x \ln\left(\sqrt{R_2^2 - x^2} + R_2\right) - x \ln\left(\sqrt{R_1^2 - x^2} + R_1\right) \end{aligned} \tag{3}$$

Since this distribution produces complex numbers for $x < R_1$, we only consider the real part of this distribution, which appears to produce a peak at $x = R_1$.

III. Results and Discussion

We found that for both the case of the spheres of constant radius, and the case of the spheres of varying radius, the experimental data reproduced a distribution in the same shape as the theoretical distribution.

We first investigated the case where we placed 750 spheres of radius 0.1 each in a cube of length 20. In this case we found that a plane in a random orientation intersects very few spheres, since the spheres are very small. The planar distribution is presented in Figure 3.

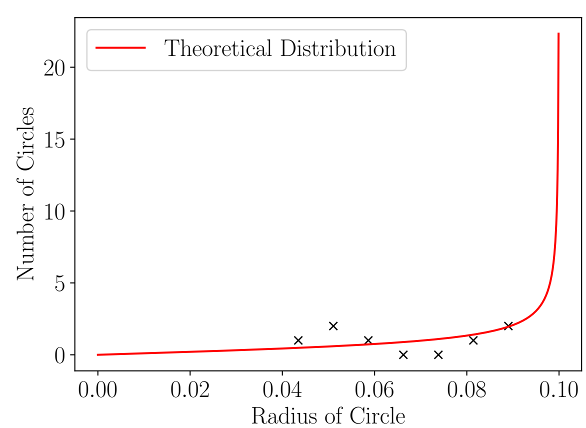


Fig. 3. Distribution of circle radii on plane for 750 spheres of radius 0.1 each. There are relatively few points since the spheres are small, so there is relatively small chance that they will be cut by the plane. So only a few circles are visible on the plane. The theoretical distribution is shown, with the experimental data matching this distribution, showing a slow increase in number or circles as radius increases.

We observe relatively few experimental data points, as there were relatively few intersections with the plane. This was likely because the spheres' radii were very small compared to box length and there were relatively few spheres. While the theoretical distribution shows a strong increase near 0.1, this is not evident from the experimental data. We also see that there is a lot of variance between the points so the slow rise evident in the theoretical distribution is not clear in the experimental data. It is thus necessary that we have more spheres that intersect with the plane, in order to obtain a larger data-set.

We found that increasing the spheres' size or placing more spheres in the box, or making the box length smaller, are all good methods of increasing the number of intersections we observe, as they all increase the likelihood of intersection by increasing the ratio of sphere occupied space to total box space. We thus next used 750 spheres of radius 0.3 each. The planar cross-sectional distribution found is presented in Figure 4.

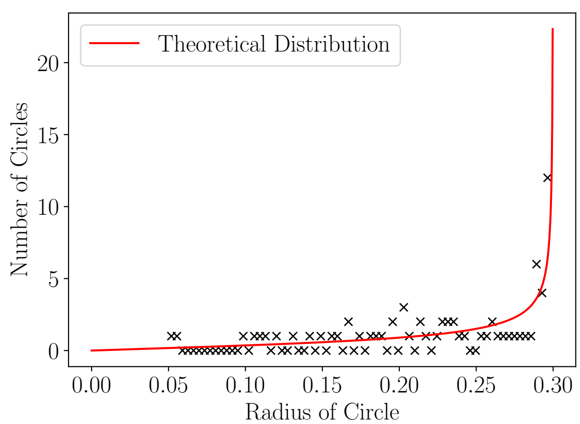


Fig. 4. Distribution of circle radii on plane for 750 spheres of radius 0.3 each. Compared to Figure 3, there are many more experimental data points, since it is more likely that the plane will intersect these larger spheres. The experimental data more clearly resembles the theoretical distribution, showing a strong increase in number of circles as radius increases towards the maximum of 0.3.

In Figure 4 we see that there are clearly more experimental data points. This is because more spheres had intersections with the plane. Compared to Figure 7b, the slow rise in the theoretical distribution is more closely followed by the experimental data. However, we still encounter significant variance and fluctuation in lower radius bins, even though the theoretical data is a smooth gradual increase. This is likely due to the relatively few number of circles populating these bins, causing greater relative difference between neighbouring bins. One method to solve this would be to use fewer bins, which would have the effect of "summing and averaging" neighbouring bins so the experimental data has a smoother trend. However, this would also reduce the number of data points so it was not implemented in our investigation.

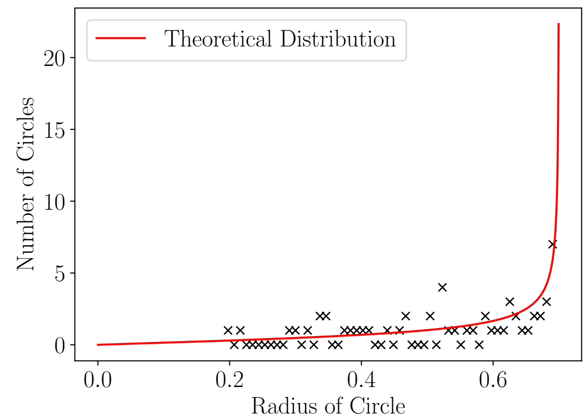


Fig. 5. Distribution of circle radii on plane for 750 spheres of radius 0.7 each. We do not observe much difference in how well the experimental data resembles the theoretical distribution between this figure and Figure 4. With larger sized spheres, the simulation becomes harder to run as it is more difficult to randomly place spheres in a finite space without overlap.

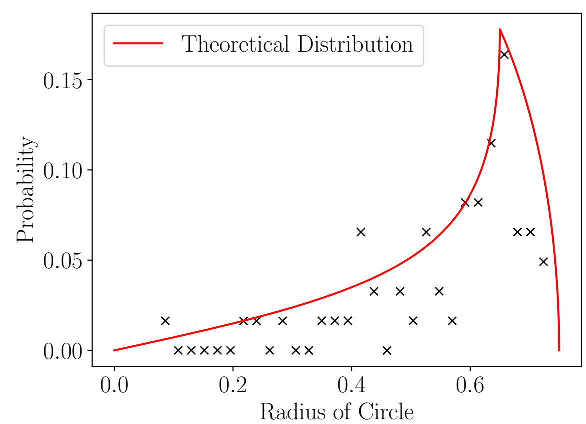
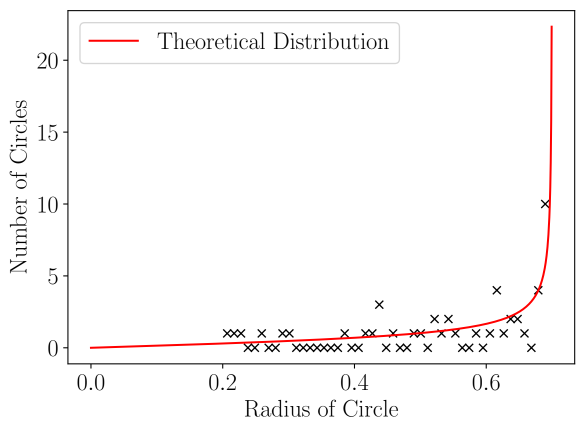


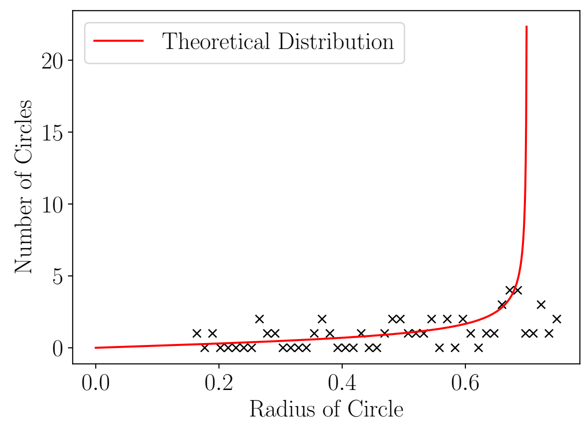
Fig. 6. Distribution of circle radii on plane for 750 spheres of radius R where $0.65 < R < 0.75$. The theoretical distribution is now different, although the experimental data still resembles this new distribution, showing a maximum around $R = 0.7$ and a sharp decrease after this. This is likely because there are more spheres with radii such that an overlap between 0 and 0.7 is possible, and relatively few spheres with radii such that a larger overlap is possible.

IV. Conclusions

Text



(a) Noise 2 orders of magnitude smaller than radius



(b) Noise 1 order of magnitude smaller than radius

Fig. 7. Distribution of circle radii on plane for 750 balls of radius 0.7 each. Each recorded radius has a random noise added to it in order to determine how sensitive the data is to experimental error. Figure 7a shows the distribution for an added noise 2 orders of magnitude smaller than the recorded radius, while Figure 7b is the same for noise 1 order of magnitude smaller. As we can see, the experimental data very resembles the theoretical distribution when noise of 2 orders of magnitude smaller are added. But this is not true when noise of 1 order of magnitude smaller is added, implying the data is very sensitive to experimental data.