

How to generate equidistributed points on the surface of a sphere

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There are two qualitatively different ways in which we could try to achieve equidistribution of points on a surface. One is to randomly place them in such a way that the probability of ending up in some particular region is proportional to the area of that region (two-dimensional Poisson statistics). This gives equidistribution *on average*. The second is to regularly place points such that their distance in two orthogonal directions is locally always the same. This gives typically a better result (no fluctuations and no accidental overlap), but the emerging partial crystallinity could sometimes be undesirable. For the case of a sphere an example for both strategies is presented.

I. SPHERICAL COORDINATES

The most straightforward way to create points on the surface of a sphere are classical spherical coordinates, in which a point is addressed via its two angular coordinates, the polar angle $\vartheta \in [0; \pi]$ and the azimuthal angle $\varphi \in [0, 2\pi]$. If the sphere has radius r , the Cartesian coordinates of that point are given by

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = r \begin{pmatrix} \sin \vartheta \cos \varphi \\ \sin \vartheta \sin \varphi \\ \cos \vartheta \end{pmatrix}. \quad (1)$$

II. RANDOM PLACEMENT

When one wants to evenly place points on the surface of a sphere, it is important to realize that it is *not* correct to simply choose the spherical angles ϑ and φ equidistributed from their permissible intervals. In order to find out what has to be done instead, it is helpful to have a look back at the area element. Notice that it can be written as

$$dA = r^2 \sin \vartheta d\vartheta d\varphi = r d(r \cos \vartheta) d\varphi = r dz d\varphi. \quad (2)$$

We thus see that it *is* correct to choose φ equidistributed from $[0; 2\pi]$ and to also choose z equidistributed from $[-r; r]$. This then gives the following algorithm for placing N randomly equidistributed points on the surface of a sphere of radius r :

```
repeat  $N$  times {
  Choose  $z$  equidistributed from  $[-r; r]$ .
  Choose  $\varphi$  equidistributed from  $[0; 2\pi]$ .
  Set  $x = \sqrt{r^2 - z^2} \cos \varphi$ .
  Set  $y = \sqrt{r^2 - z^2} \sin \varphi$ .
}
```

The result of such an algorithm is illustrated in Fig. 1a.

III. REGULAR PLACEMENT

Regular equidistribution can be achieved by choosing circles of latitude at constant intervals d_ϑ and on these

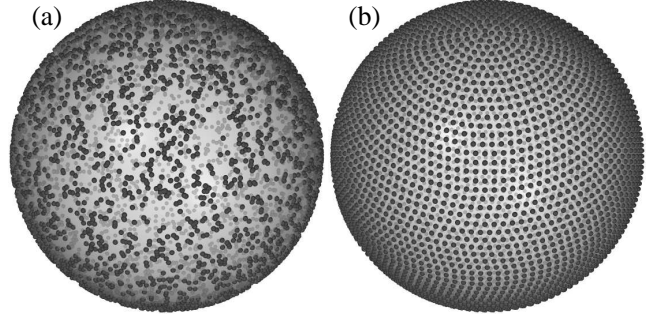


FIG. 1: Illustration of the two algorithms for putting points equidistributed onto the surface of a sphere discussed in these notes. In both cases $N = 5000$, case (a) is the random placement, case (b) the regular one. In the latter the algorithm actually could only place 4999 points.

circles points with distance d_φ , such that $d_\vartheta \simeq d_\varphi$ and that $d_\vartheta d_\varphi$ equals the average area per point. This then gives the following algorithm:

```
Set  $N_{\text{count}} = 0$ .
Set  $a = 4\pi r^2 / N$  and  $d = \sqrt{a}$ .
Set  $M_\vartheta = \text{round}[\pi/d]$ .
Set  $d_\vartheta = \pi/M_\vartheta$  and  $d_\varphi = a/d_\vartheta$ .
For each  $m$  in  $0 \dots M_\vartheta - 1$  do {
  Set  $\vartheta = \pi(m + 0.5)/M_\vartheta$ .
  Set  $M_\varphi = \text{round}[2\pi \sin \vartheta / d_\varphi]$ .
  For each  $n$  in  $0 \dots M_\varphi - 1$  do {
    Set  $\varphi = 2\pi n / M_\varphi$ .
    Create point using Eqn. (1).
     $N_{\text{count}} += 1$ .
  }
}
```

At the end of this algorithm N_{count} points have been placed, with N_{count} very close to N . The result of such an algorithm is illustrated in Fig. 1b.

Note that the regular placement is far more even: neither local clustering (points almost sitting on top of each other) nor global \sqrt{N} fluctuations occur. For setting up a liquid state the second algorithm thus appears more favorable.