

On the, not entirely trivial, issue of getting uniformly distributed random coordinates within a sphere.

H. T. Ihle

The rand-functions in c++ can give us random numbers uniformly distributed between 0 and 1. But we need somehow to convert these numbers into coordinates of uniformly distributed particles within a sphere of radius R_0 .

The easy way to do this would be to get a uniform distribution of particles in a cube of volume $(2R_0)^3$, and then just throw away all the particles outside the sphere, but this is not very satisfying. A more elegant way to do this is to use spherical coordinates.

$$x = r \sin \theta \cos \phi \tag{1}$$

$$y = r \sin \theta \sin \phi \tag{2}$$

$$z = r \cos \theta \tag{3}$$

$$\theta \in [0, \pi], \phi \in [0, 2\pi], r \in [0, R_0].$$

The problem is, it is not obvious how to get a uniform density of particles. If we distribute the particles uniformly in r , the density will be much higher in the centre. And if we distribute the particles uniformly in θ they will clump towards the poles.

There is a easy trick to solve this problem, we can use the fact that the volume element should be the same for any coordinate system. If we introduce three new variables with a uniform distribution between 0 and 1 we can write the volume element in terms of these coordinates, and tie each coordinate to one of the spherical coordinates. We get

$$r^2 \sin \theta dr d\theta d\phi = A du dv dw,$$

where A is just a constant and $u, v, w \in [0, 1]$. If we separate the coordinates we get three equations

$$r^2 dr = a du, \sin \theta d\theta = b dv, d\phi = c dw,$$

where a, b, c are just constants obeying $A = abc$.

Lets start with the easy one and just integrate up,

$$d\phi = c dw \Rightarrow \quad (4)$$

$$\phi = c w \Rightarrow \quad (5)$$

$$2\pi = c, \quad (6)$$

where we have used that $\phi = 2\pi$ corresponds to $w = 1$.

Lets go on using the same approach

$$r^2 dr = a du \Rightarrow \quad (7)$$

$$\int_0^r r'^2 dr' = a \int_0^u du' \Rightarrow \quad (8)$$

$$\frac{1}{3} r^3 = a u \Rightarrow \quad (9)$$

$$\frac{1}{3} R_0^3 = a, \quad (10)$$

$$r = \sqrt[3]{3 \frac{1}{3} R_0^3 u} \Rightarrow \quad (11)$$

$$r = R_0 \sqrt[3]{u}. \quad (12)$$

Confident that we are on the right track we go on to the last case

$$\sin \theta d\theta = b dv \Rightarrow \quad (13)$$

$$\int_0^\theta \sin \theta' d\theta' = b \int_0^v dv' \Rightarrow \quad (14)$$

$$1 - \cos \theta = b v \Rightarrow \quad (15)$$

$$2 = b, \quad (16)$$

$$\theta = \arccos(1 - 2v). \quad (17)$$

Thus if we now let our random numbers (between 0 and 1) represent the value of the three coordinates u, v, w , we can get values for the spherical coordinates. We can then use these to get back to the cartesian coordinates we want.