

# Distribution of particles into ScalFMM

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# 1 Uniform distribution for surface

For parametric surface, J Williamson in [1] proposed a method to construct uniform distribution of points on such surface. For ellipsoid, this method was improved in [2]. Here we follow their approach to construct uniform distribution.

## 1.1 Sphere distribution

Consider that we want  $N$  point uniformly set on the surface of the unit sphere, the natural choice is to sample uniformly the angles  $\theta$  and  $\phi$  of the spherical coordinates. Unfortunately, such choice lead to a concentration of points near the pole. As a surface area is given by  $\sin\phi d\phi d\theta = -d(\cos\phi) d\theta$ , we will sample  $\cos\phi$  rather than  $\Phi$ . So, we choose  $u$  and  $v$  two random variable on  $[0,1]$  and

$$\begin{aligned}\theta &= 2\pi u, \\ \phi &= \cos^{-1}(2v - 1).\end{aligned}$$

then we obtain a uniform distribution of points on the unit sphere.

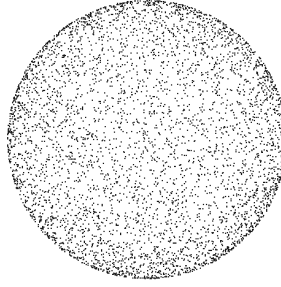


Figure 1: 5 000 points distribution on unit sphere.

```
generateDistributions -unitsphere -N 5000 -fout unitsphere.fma -fvisuout unitsphere.vtp
```

## 1.2 Ellipsoid distribution

Here we want to construct a uniform distribution on an ellipsoid defined by the equation

$$f(x, y, z) = \left(\frac{x}{a}\right)^2 + \left(\frac{y}{b}\right)^2 + \left(\frac{z}{c}\right)^2 - 1, \quad (1)$$

and the parameterization

$$\begin{aligned}x &= a \cos(u) \cos(v), \\ y &= b \cos(u) \sin(v), \\ z &= c \sin(u).\end{aligned}$$

with  $u \in [0, 2\pi[$  and  $v \in [0, \pi[$ . if you sample  $u$  and  $v$  then we obtain a non uniform distribution on the ellipsoid see section 2.1.

### 1.2.1 prolate

A prolate spherical geometry is an ellipsoid where  $a = b$  and  $c > a$ . On the case  $g_{max} = 1 + a^2$  is obtain when  $z = o$ . Then to construct a uniform distribution we proceed as follow

**step 1** Build a uniform point on the sphere and map it on the prolate surface. Let  $u$  a random point in  $[-1, 1]$  and  $v$  in  $[0, \pi]$ , then

$$\begin{aligned}x &= a\sqrt{1-u^2}\cos(v), \\y &= b\sqrt{1-u^2}\sin(v), \\z &= cu.\end{aligned}$$

**step 2** Correct the distribution. Choose a random point  $\xi$  in  $[0, 1]$  and if

$$x^2 + y^2 + \frac{a^4}{c^4}z^2 < a^2\xi^2$$

is true then we keep the point otherwise we reject it.

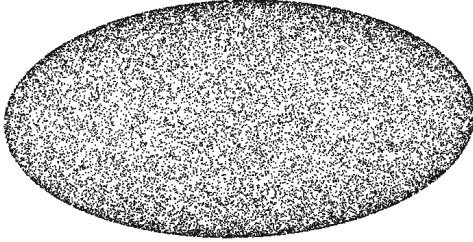


Figure 2: 20 000 points distribution on 2:2:4 ellipsoid. Less than 15% of points has been rejected.

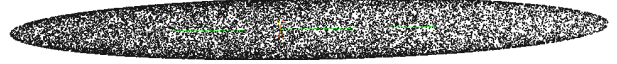


Figure 3: 20 000 points distribution on 1:1:10 ellipsoid and only 21% of the tested points in step 2 has been rejected.

```
generateDistributions -prolate -ar 1:1:10 -N 20000 -fout prolate.bfma -fvisuout
prolate.vtp
```

## 2 Non uniform distribution

### 2.1 Ellipsoid

The simplest way to sample an ellipsoid of size  $a:b:c$  is to consider its spherical coordinates. Let  $u$  and  $v$  two random numbers between 0 and 1. After mapping  $u$  (resp.  $v$ ) in  $[-\pi/2, \pi/2]$  (resp.  $[-\pi, \pi]$ ), the Cartesian coordinates are

$$\begin{aligned}x &= a\cos(u)\cos(v), \\y &= b\cos(u)\sin(v), \\z &= c\sin(u).\end{aligned}$$

As shown in the figure 4 we obtain a concentration of points near the poles  $(0, 0, \pm c)$ . This bias on the pole could be reduced by choosing the same approach that we use to build a uniform distribution on the unit sphere?

```
generateDistributions -ellipsoid -ar 2:2:4 -N 20000 -fout ellipsoid.bfma -fvisuout
ellipsoid.vtp
```

If you consider the

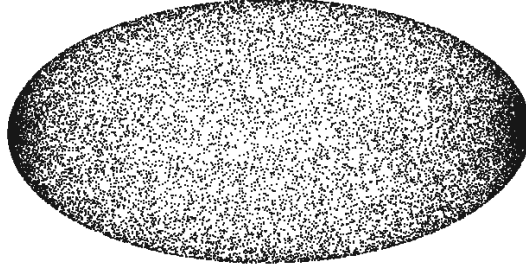


Figure 4: 20 000 points distribution on an ellipsoid of aspect ratio 2:2:4.

## 2.2 Plummer Model

This is a hard test case in astrophysics problem, and it models a globular cluster of stars, which is highly non uniform. It is called the plummer distribution. To construct such distribution, first we construct a uniform points distribution on the unit sphere. Second, the radius is chosen according to the plummer distribution (double power law in astrophysics). We consider  $u$  a random number between 0 and 1, then the associated radius is given by

$$r = 1.0 / \sqrt{u^{-2/3} - 1}$$

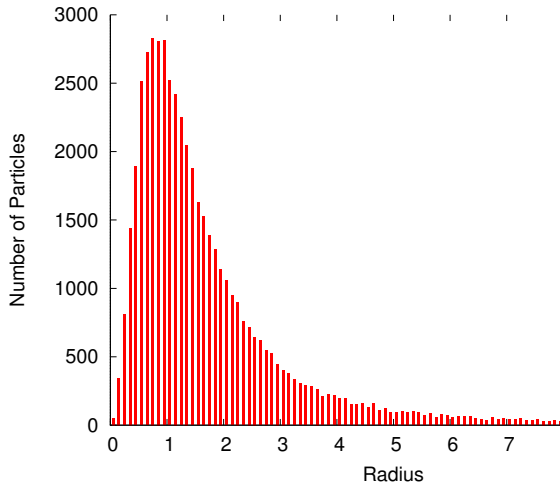


Figure 5: Radius distribution

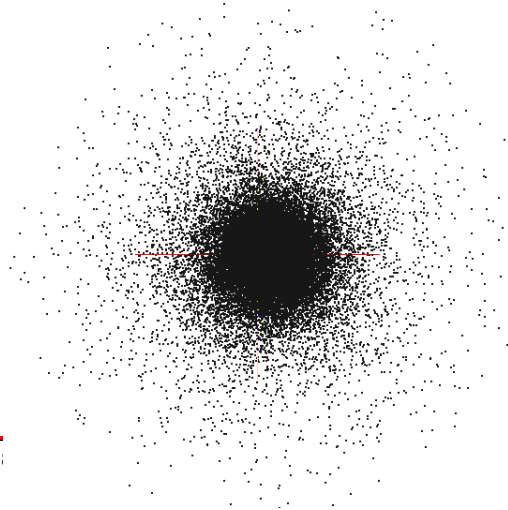


Figure 6: 50 000 point distribution.

The command to generate such distribution is  
`generateDistributions -plummer -radius 10 -N 50000 -fout plummer.bfma -fvisuout plummer.vtp`

The Plummer 3-dimensional density profile is

$$\rho_P(r) = \frac{3M}{4\pi a^3} \left(1 + \frac{r^2}{a^2}\right)^{-\frac{5}{2}} \quad (2)$$

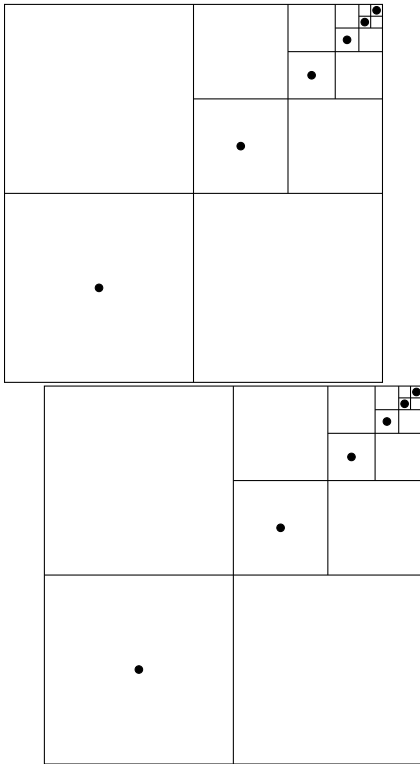
where  $M$  is the total mass of the cluster and  $a$  the Plummer radius.

The corresponding potential is

$$\Phi_P(r) = -\frac{GM}{\sqrt{r^2 + a^2}} \quad (3)$$

In N-body units,  $G = M = 1$  and  $a = 3\pi/16 \sim 0.589$

## 2.3 Diagonal Model



## References

- [1] J. F. Williamson, Random selection of points distributed on curved surfaces, *Physics in Medicine and Biology*, vol. 32, no. 10, pp. 1311-1319, Oct. 1987.
- [2] T. Chen and S. C. Glotzer, Simulation studies of a phenomenological model for elongated virus capsid formation, *Physical review. E, Statistical, nonlinear, and soft matter physics*, vol. 75, pp. 125, 2007.

## 3 Annexe

### 3.1 Gnuplot script for histogram

```
clear
reset
set key off
set border 3
# Add a vertical dotted line at x=0 to show centre (mean) of distribution.
set yzeroaxis

# Each bar is half the (visual) width of its x-range.
set boxwidth 0.05 absolute
set style fill solid 1.0 noborder

bin_width = 0.1;

bin_number(x) = floor(x/bin_width)

rounded(x) = bin_width * ( bin_number(x) + 0.5 )

set xlabel "Radius"
set ylabel "Number of Particles"

#set terminal postscript enhanced color 'Helvetica' 20
#set output 'plummerHistogramme.eps'

plot 'plummerNewSort.txt' using (rounded($1)):(1) smooth frequency with boxes
```