Distribution of particles into ScalFMM

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Version 0.1

Contents

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 θ and ϕ 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 Φ. 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.

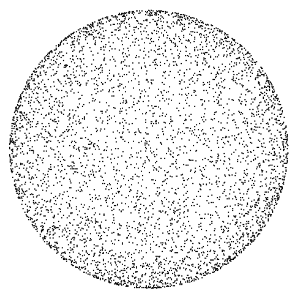


Figure 1: 5 000 points distribution on unit sphere.

```
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

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

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 ξ 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.

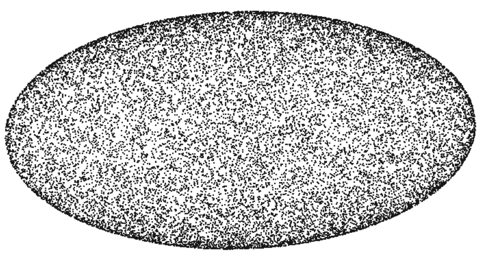


Figure 2: 20 000 points distribution on 2:2:4 ellipsoid. Less than 15% of points has been rejected.

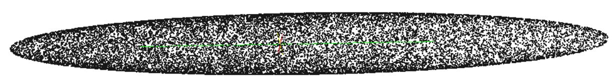


Figure 3: 20 000 points distribution on 1:1:10 ellipsoid and only 21% of the tested points in step 2 has been rejected.

```
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 and 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

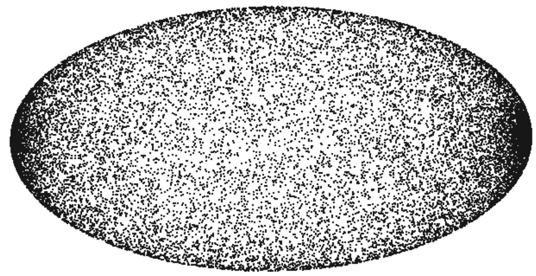


Figure 4: 20 000 points distribution on an ellipsoid of aspect ratio 2:2:4.

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

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

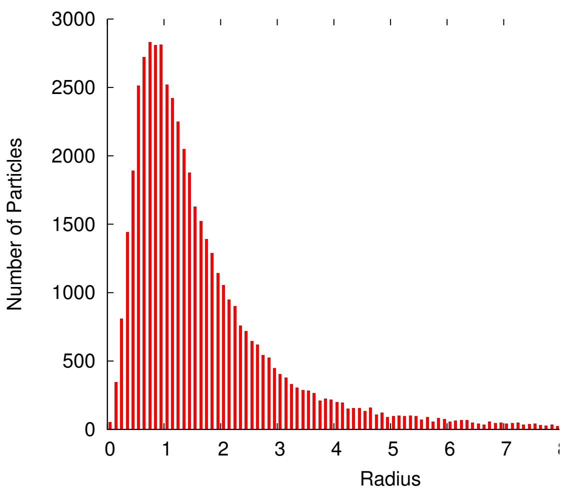


Figure 5: Radius distribution

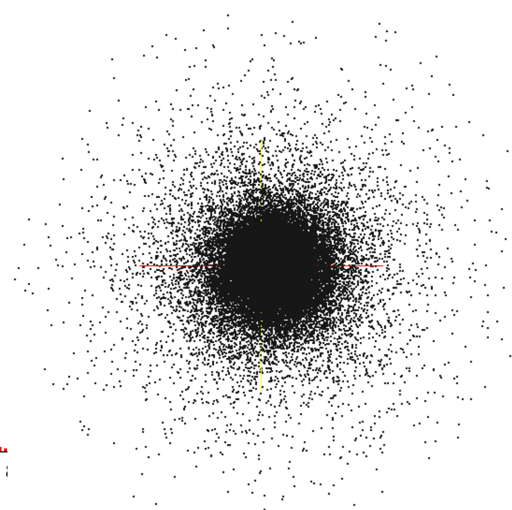


Figure 6: 50 000 point distribution.

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

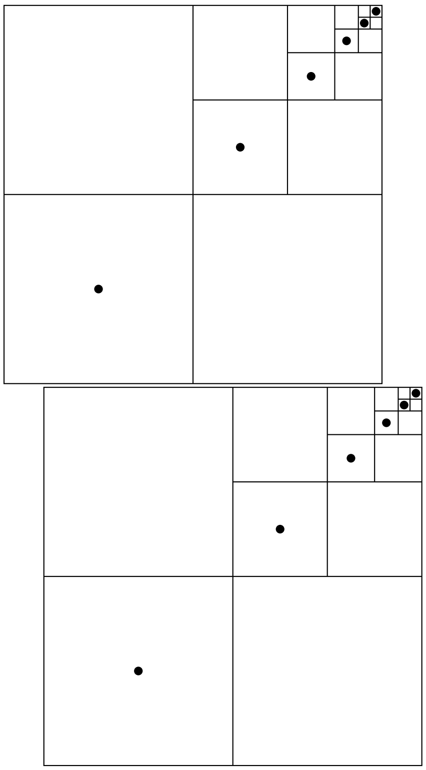
$$\rho_P(r) = \frac{3M}{4\pi a^3}(1 + \frac{r^2}{a^2})^{-\frac{5}{2}} \tag{2}$$

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

The corresponding potential is

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

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. 13111319, 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
```