

SAMPLING SPECIAL DISTRIBUTIONS

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1. INTRODUCTION

Monte Carlo simulations require the sampling of various distributions at different steps in the simulation process. There exist a multitude of approximate algorithms that have been ingeniously devised to sample some specified functions. In other cases special geometrical sources need to be sampled for starting up the solution or to account for the boundary or initial conditions.

Sampling these distributions adequately depends upon correctly identifying the underlying probability density functions, deducing the corresponding cumulative distribution functions, and next inverting them to sample the source, the boundary or the initial condition. Several geometric sources are considered to demonstrate the approach.

2. SAMPLING ISOTROPIC SOURCES

We consider the sampling of an isotropic spherically symmetric source of particles or photons. In this case each element of solid angle receives the same contribution from the isotropic source as shown in Fig. 1. This means we have to sample the probability density function in spherical coordinates:

$$\begin{aligned} p(\theta, \phi)d\theta d\phi &= \frac{d\Omega}{4\pi} = \frac{dS}{4\pi r^2} \\ &= \frac{r^2 \sin\theta d\theta d\phi}{4\pi r^2} \\ &= \frac{\sin\theta d\theta}{2} \cdot \frac{d\phi}{2\pi} \end{aligned} \quad (1)$$

where: the element of solid angle $d\Omega = \frac{dS}{r^2}$.

Here the probability density function is separable into two probability density functions:

$$p(\theta, \phi)d\theta d\phi = p(\theta)d\theta \cdot p(\phi)d\phi$$

where:

$$p(\theta)d\theta = \frac{\sin\theta d\theta}{2}, \quad \int_0^\pi \frac{\sin\theta}{2} d\theta = 1 \quad (2)$$

$$p(\phi)d\phi = \frac{d\phi}{2\pi}, \quad \frac{1}{2\pi} \int_0^{2\pi} d\phi = 1 \quad (3)$$

These probability density functions represent two independent random variables, and can be sampled separately. Setting:

$$C(\phi) = \int_0^{\phi} \frac{d\phi}{2\pi} = \rho_1, \quad (4)$$

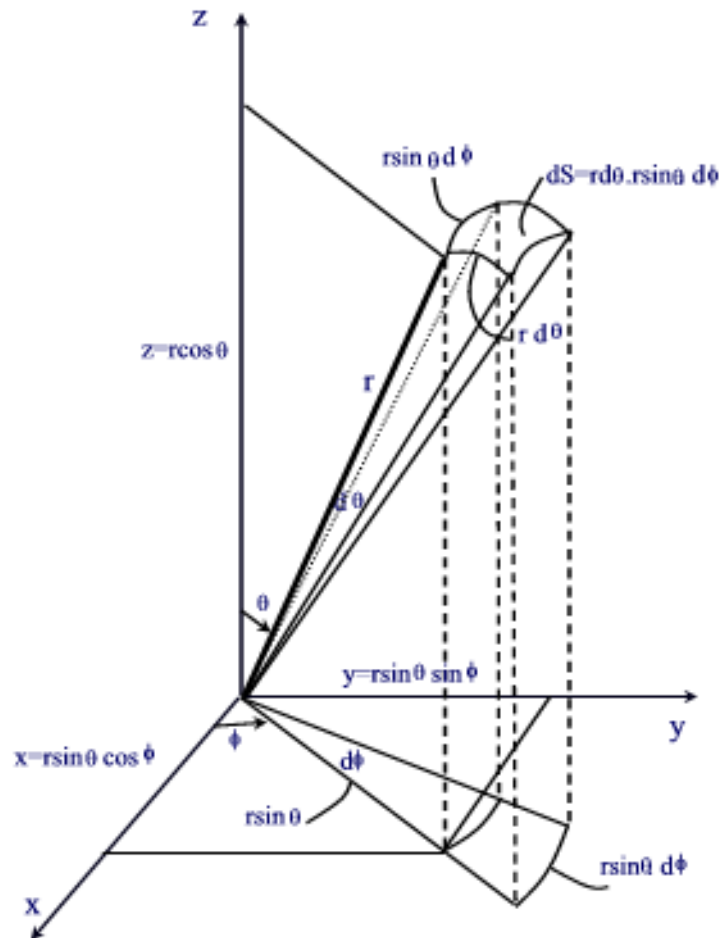


Figure 1. Sampling an isotropic spherically symmetric source.

we can sample the azimuthal angle from:

$$\phi(\rho) = 2\pi\rho_1 \quad (5)$$

Setting:

$$C(\theta) = \int_0^\theta \frac{\sin \theta}{2} d\theta = \rho_2,$$

$$1 - \cos \theta = 2\rho_2,$$

$$\cos \theta = 1 - 2\rho_2.$$

or the polar angle can be sampled as:

$$\theta = \cos^{-1}(1 - 2\rho_2) \quad (6)$$

Now that the polar and azimuthal angles have been sampled, we can determine the direction cosines u , v , and w for the particles or photons emanating from the isotropic source according to the simple relationships:

$$\begin{aligned} u &= \frac{x}{r} = \frac{r \sin \theta \cos \phi}{r} = \sin \theta \cos \phi \\ v &= \frac{y}{r} = \frac{r \sin \theta \sin \phi}{r} = \sin \theta \sin \phi \\ w &= \frac{z}{r} = \frac{r \cos \theta}{r} = \cos \theta \end{aligned} \quad (7)$$

An alternate form of this sampling scheme can be advanced by defining:

$$\mu = \cos \theta$$

Using the Pythagorean Theorem, we can write:

$$\sin \theta = \sqrt{1 - \cos^2 \theta} = \sqrt{1 - \mu^2}$$

This leads to an alternate form of Eqn. 7 as:

$$\begin{aligned} u &= \sqrt{1 - \mu^2} \cdot \cos \phi \\ v &= \sqrt{1 - \mu^2} \cdot \sin \phi \\ w &= \mu \end{aligned} \quad (7)'$$

3. SAMPLING THE NORMAL OR GAUSSIAN DISTRIBUTION

Invoking the Central Limit Theorem one can generate a Normal or Gaussian variable, also called a Bell Curve, in terms of a sequence of pseudo random variables uniformly distributed over the unit interval. For such a random variable the mean value, mathematical expectation or simply first moment of the distribution is:

$$\mu = \frac{\int_0^1 xf(x)dx}{\int_0^1 f(x)dx} = \frac{\int_0^1 x.1.dx}{\int_0^1 1.dx} = \left[\frac{x^2}{2}\right]_0^1 = \frac{1}{2}, \quad (8)$$

and the variance is:

$$\sigma^2 = \frac{\int_0^1 x^2 f(x)dx}{\int_0^1 f(x)dx} - \mu^2 = \frac{\int_0^1 x^2.1.dx}{\int_0^1 1.dx} - \mu^2 = \left[\frac{x^3}{3}\right]_0^1 - \left(\frac{1}{2}\right)^2 = \frac{1}{3} - \frac{1}{4} = \frac{1}{12}, \quad (9)$$

Thus its standard deviation is:

$$\sigma = \frac{1}{\sqrt{12}} \quad (10)$$

According to the Central Limit Theorem, the random variable:

$$\xi = \frac{\sum_{i=1}^n x_i - n\mu}{\sqrt{n}\sigma} \quad (11)$$

converges asymptotically with n to a Normal distribution with mean μ and variance σ^2 :
N(μ , σ):

$$N(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{\left[-\frac{(x-\mu)^2}{2\sigma^2}\right]}, \quad -\infty < x < \infty \quad (12)$$

For the sampling of a uniform random distribution, we can substitute from Eqs. 9 and 11 for the values of the mean and standard deviation as:

$$\xi = \frac{\sum_{i=1}^n r_i - \frac{n}{2}}{\sqrt{\frac{n}{12}}} \quad (13)$$

As a good approximation, we can take n = 12 in Eqn. 13 to yield:

$$\xi = \sum_{i=1}^{12} r_i - 6 \quad (14)$$

which yields a very simple algorithm to generate a Normal or Gaussian variate:

1. Generate a sequence of 12 random numbers r_i , $i=1, 2, \dots, 12$, over the unit interval.
2. Let: $\xi = \sum_{i=1}^{12} r_i - 6$,
3. Report a sample: $\xi' = \mu + \xi\sigma$ from $N(\mu, \sigma^2)$.

Sometimes the 90 percent error spread factor is used instead of the standard deviation as a parameter:

$$\xi' = \mu + \xi(1.645\sigma).$$

A procedure that generates a Normal random variable by the above-mentioned algorithm is shown in Fig. 2. It uses calls to a subroutine to reconstruct a Normal variable that is displayed in Fig. 3.

```

!      normal_gaussian_distribution.f90
!      Sampling the Normal or Gaussian distribution
!      M. Ragheb
      program normal_gaussian_distribution
      dimension e(100), freq(100)
      integer :: trials = 100000
      real x, e, freq, score
      real :: xmean =10.0
      real :: std_dev = 3.0
      score = 1.0
! Initialize frequency distribution
      do i=1,20
          freq(i)=0.0
      end do
! Initialize bins
      do i=1,20
          xi=i
          e(i)=xi
      end do
! open output file
      open(44, file = 'random_out')
! Sample distribution
      do i= 1, trials
! Sample x coordinate
          call normal(xmean,std_dev,x,rr)
! Construct frequency distribution
          if(x.LE.e(1))then
              freq(1)=freq(1)+score
          end if
          do j=1,20
              if((x.GT.e(j)).AND.(x.LE.e(j+1)))then
                  freq(j+1)=freq(j+1)+score
              end if
          end do
      end do

```

```

    end do
!   Normalize frequency distribution and construct pdf
    do i=1,20
        freq(i)=freq(i)/trials
    end do
!   Write results to output file
    do i=1,20
        write (44,100)e(i),freq(i)
        write(*,*)e(i),freq(i)
    end do
100  format (2e14.8)
    end

    subroutine normal(xmean,std_dev,x,rr)
!   This subroutine generates a Normal or Gaussian random variable
!   with a mean value xmean and a standard deviation std_dev
!   mean value= xmean
!   standard deviation= std_dev
!   returned sampled point= x
!   90% error spread= s = 1.645*standard deviation
    n=12
    xn=n
!   s=1.645*std_dev
    s=std_dev
    const = sqrt (xn/12.0)
    sum = 0.0
    do i=1,n
        call random(rr)
        sum = sum + rr
    end do
    v=(sum-(xn/2.0))/const
    x=xmean + v*s
    return
    end

```

Figure 2. Procedure for sampling and displaying the Normal or Gaussian distribution.

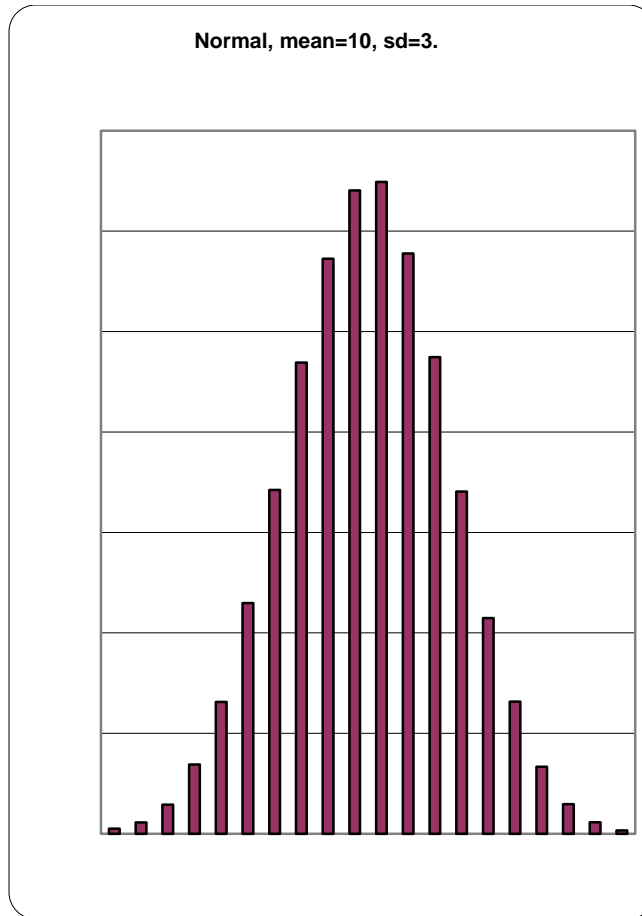


Figure 3. Sampled Normal or Gaussian distribution, N=100,000 trials.

4. SAMPLING THE LOGNORMAL DISTRIBUTION

A distribution related to the Normal distribution is the Lognormal or Logarithmico-Normal distribution. If X is from $N(\mu, \sigma^2)$, then $Y = e^X$ has the Lognormal distribution with a pdf:

$$f_Y(y) = \frac{1}{\sqrt{2\pi}\sigma y} e^{\left[-\frac{(\ln y - \mu)^2}{2\sigma^2}\right]}, \quad 0 < y < \infty \quad (15)$$

An algorithm based on the Central Limit Theorem can thus be proposed to generate the Lognormal distribution:

1. Generate a sequence of 12 random numbers r_i , $i = 1, 2, \dots, 12$, over the unit interval.
2. Let: $\xi = \sum_{i=1}^{12} r_i - 6$,

3. Generate a sample: $X = \mu + \xi\sigma$ from $N(\mu, \sigma^2)$.
4. Report $Y = e^X$ as a sample from the Lognormal distribution.

A procedure using this algorithm is shown in Fig. 4, where a subroutine is called to generate the samples, and the ensuing Lognormal distribution is shown in Fig. 5.

```

!      lognormal_distribution f90
!      Sampling the lognormal distribution
!      M. Ragheb
program lognormal_distribution
dimension e(101), freq(101)
integer :: trials = 1000000
real x, e, freq, score
real :: xmean =20.0
real :: std_dev = 3.0
score = 1.0
!      Initialize frequency distribution
do i=1,100
        freq(i)=0.0
end do
!      Initialize bins
do i=1,100
        xi=i
        e(i)=xi
end do
!      open output file
open(44, file = 'random_out')
!      Sample distribution
do i= 1, trials
!      Sample x coordinate
        call lognormal(xmean,std_dev,x,rr)
!      Construct frequency distribution
        if(x.LE.e(1))then
            freq(1)=freq(1)+score
        end if
        do j=1,100
            if((x.GT.e(j)).AND.(x.LE.e(j+1)))then
                freq(j+1)=freq(j+1)+score
            end if
        end do
end do
!      Normalize frequency distribution and construct pdf
do i=1,100
        freq(i)=freq(i)/trials
end do
!      Write results to output file
do i=1,100
        write (44,100)e(i),freq(i)
        write(*,*)e(i),freq(i)
end do
100 format (2e14.8)
end

subroutine lognormal(xmean,std_dev,x,rr)
!      This subroutine generates a Lognormal random variable
!      from a normal distribution with zero mean and unit standard
!      deviation
!      mean value= xmean
!      standard deviation= std_dev
!      returned sampled point= x

```



```

!      90% error spread = s = 1.645*standard deviation
      n=12
      xn=n
      xxmean= alog (xmean)
      sstd_dev = alog (std_dev)
!      s=1.645*std_dev
      s=sstd_dev
      const = sqrt (xn/12.0)
      sum = 0.0
      do i=1,n
          call random(rr)
          sum = sum + rr
      end do
      v=(sum-(xn/2.0))/const
      xx=xxmean + v*s
      x=exp(xx)
      return
      end

```

Figure 4. Procedure for the sampling and displaying the lognormal distribution.

5. SAMPLING LINE SOURCES

Sampling different source geometrical configurations is encountered in many problems such as shielding against radiation, fluid flow and heat transport problems. It depends upon correctly identifying the underlying probability density function, deducing the corresponding cumulative distribution function and then inverting it to sample the source. Several geometries are encountered in practice. We consider the most important ones of them to demonstrate the approach to sampling them.

The probability density function for a line source of length H along the z coordinate axis can be written as:

$$pdf : f(z)dz = \frac{dz}{\int_0^H dz} = \frac{dz}{H} \quad (16)$$

Notice the normalization in the denominator. The geometry used in the sampling is shown in Fig. 6.

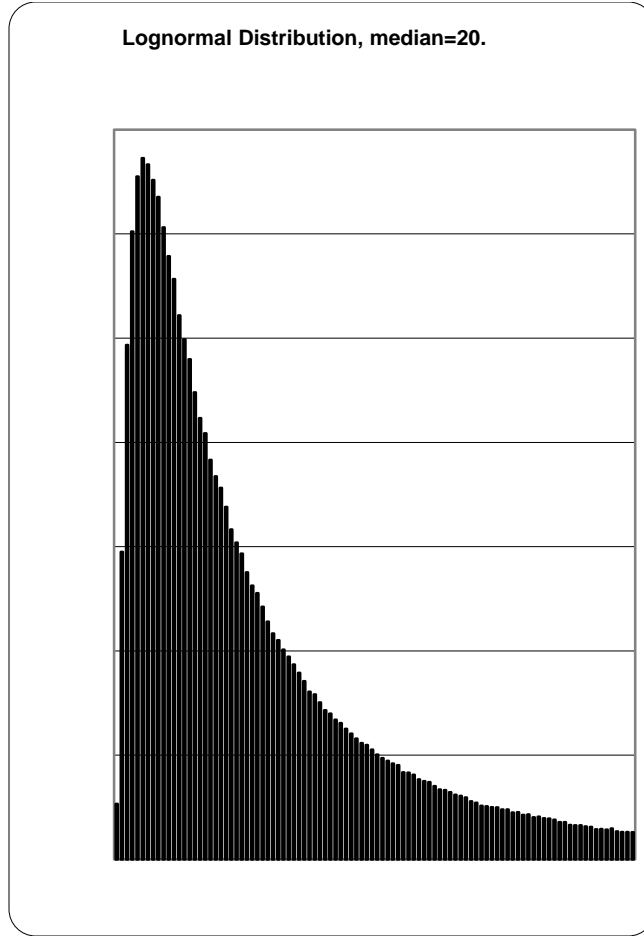


Figure 5. A sampled lognormal distribution with median $M = 20$.

The cumulative distribution function is:

$$cdf : C(z) = \frac{\int_0^z dz}{H} = \frac{z}{H} = \rho \quad (17)$$

Equating the cdf to a pseudo random number uniformly distributed over the unit interval allows us to sample the positions along the line source in a straightforward way as:

$$z = H\rho \quad (18)$$

6. SAMPLING A DISK SOURCE

Considering a disk centered at the origin with radius R , we can deduce its pdf and the cdf, as shown in Fig. 7, as a function of the radius r as:

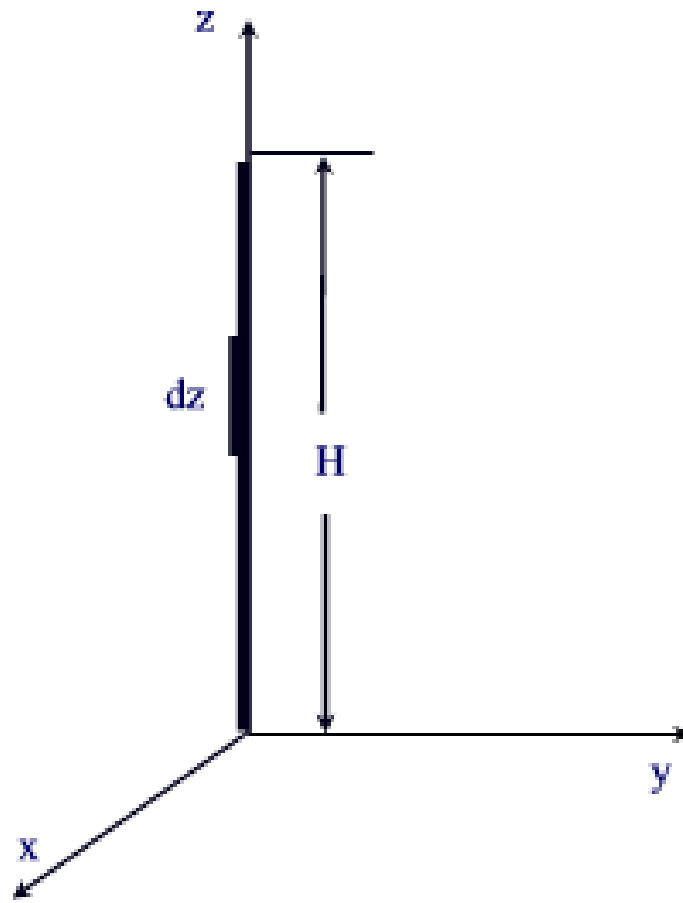


Figure 6. Line Source geometry.

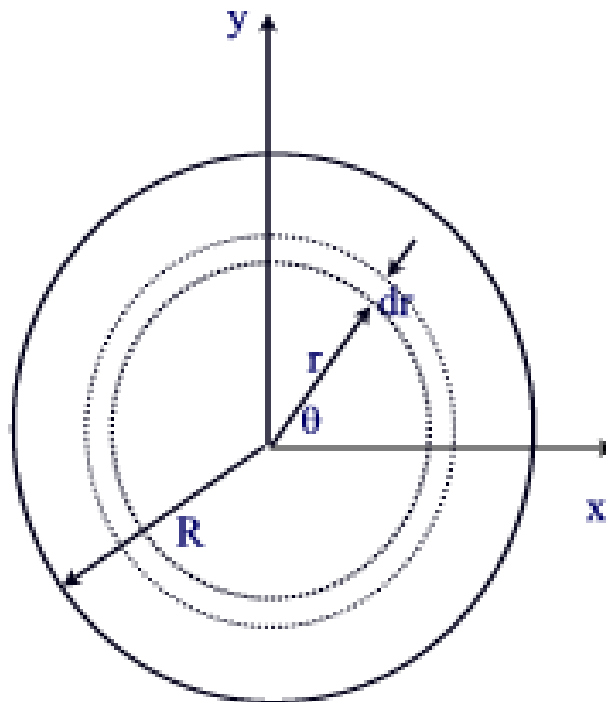


Figure 7. Disk Source geometry.

```

!      disk_source f90
!      Sampling sources uniformly distributed on a disk of radius R
!      pdf = f(r) = 2*pi*r / pi*R**2
!      cdf = C(r) = r**2/R**2
!      pdf = f(phi) = 1/(2*pi)
!      cdf      = C(phi) = phi/(2*pi)
!      M. Ragheb
!      program disk_source
!      Variables declaration
!      real :: radius = 1.0
!      real :: pi = 3.14159
!      integer :: trials = 1000
!      real r, phi, x, y
!      Open output file
!      open(44, file = 'random_out')
!      Begin sampling points
!      do i= 1, trials
!      Sample radius on disk
!      call random(rr)
!      r= radius * sqrt (rr)

```

```

!      Alternate source sampling
!      r=radius * rr
!      Sample azimuthal angle
!      call random(rr)
!      phi = 2.0*pi*rr
!      Calculate x and y coordinates
!      x = r * cos (phi)
!      y = r * sin (phi)
! Write sampled points to output file
!      write (44,100) x, y
!      write(*,*) x, y
!      format (2e14.8)
100
      end do
end

```

Figure 8. Disk source sampling procedure.

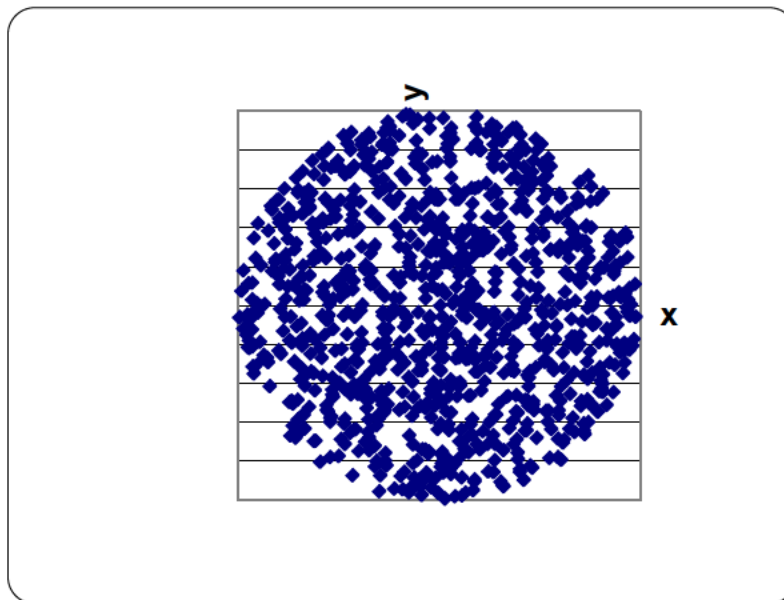


Figure 9. Uniformly distributed source on a unit radius disk. N=1,000.

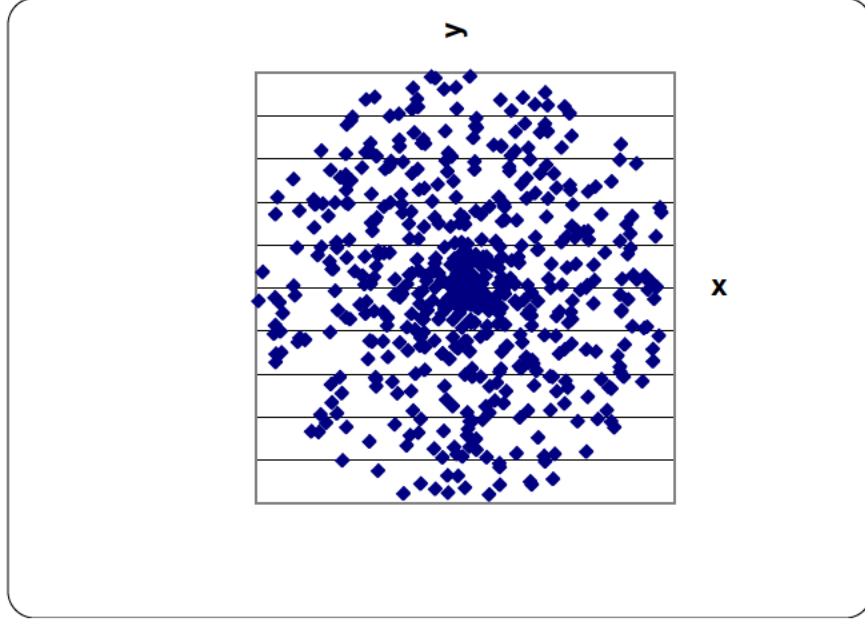


Figure 10. Incorrectly sampled distributed source on a unit radius disk. $N=1,000$.

$$pdf : f(r)dr = \frac{dA}{\int dA} = \frac{2\pi r dr}{\int_0^R 2\pi r dr} = \frac{2\pi r dr}{\pi R^2} \quad (19)$$

$$cdf : C(r) = \frac{\int_0^r 2\pi r dr}{\pi R^2} = \rho_1 \quad (20)$$

Which can be inverted to sample the radius r as:

$$r = R\rho_1^{1/2} \quad (21)$$

For the angle θ we can write the pdf and cdf:

$$pdf : f(\theta)d\theta = \frac{d\theta}{\int_0^{2\pi} d\theta} = \frac{d\theta}{2\pi} \quad (22)$$

$$cdf : C(\theta) = \frac{\int_0^\theta d\theta}{2\pi} = \frac{\theta}{2\pi} = \rho_2 \quad (23)$$

Inverting the cdf we get the sampled angle as;

$$\theta = 2\pi\rho_2 \quad (24)$$

Notice that we needed here to generate two pseudo random numbers for the radius and angular variables. The x and y coordinates for a point on the disk can thus be deduced as:

$$x = r \cos \theta = R\rho_1^{1/2} \cos(2\pi\rho_2) \quad (25)$$

$$y = r \sin \theta = R\rho_1^{1/2} \sin(2\pi\rho_2) \quad (26)$$

We could have opted to sample the angle θ over the interval $[-\pi, +\pi]$. In this case we choose:

$$\theta' = \pi(2\rho_2 - 1) \quad (27)$$

since the cdf is this case:

$$cdf : C(\theta') = \frac{\int_{-\pi}^{\theta'} d\theta'}{2\pi} = \frac{\theta' + \pi}{2\pi} = \rho_2 \quad (28)$$

Figure 8 shows a procedure for sampling a disk source. The uniform source sampled with 1,000 points is shown in Fig. 9. If one had chosen the source as proportional to the pseudo random number rather than its square root, an incorrect nonuniform source would have ensued as shown in Fig. 10. This shows a possible pitfall in the setting of a sampling scheme.

7. SAMPLING A RING SOURCE

This can be considered as a special case of the disk source with pdf and cdf for the radial parameter r as:

$$pdf : f(r)dr = \frac{dA}{\int_{R_1}^{R_2} dA} = \frac{2\pi r dr}{\int_{R_1}^{R_2} 2\pi r dr} = \frac{2\pi r dr}{\pi(R_2^2 - R_1^2)} \quad (29)$$

where R_1 and R_2 are the inner and outer radii of the ring respectively, as shown in Fig. 11.

$$cdf : C(r) = \frac{\int_{R_1}^r 2\pi r dr}{\pi(R_2^2 - R_1^2)} = \frac{\pi(r^2 - R_1^2)}{\pi(R_2^2 - R_1^2)} = \rho \quad (30)$$

By inversion we can sample the radius r on the ring as:

$$\begin{aligned} r^2 &= R_1^2 + (R_2^2 - R_1^2)\rho \\ r &= [R_1^2 + (R_2^2 - R_1^2)\rho]^{1/2} \end{aligned} \quad (31)$$

The sampling of the angular variable would be the same as in the case of the disk source.

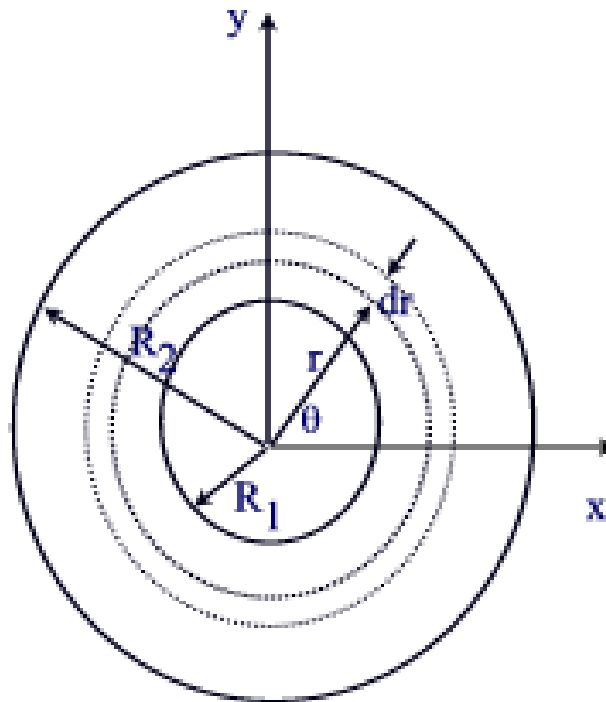


Figure 11. Ring Source geometry.

```
! ring_source f90
! Sampling sources uniformly distributed on a disk of radius R
! pdf = f(r) = 2*pi*r / pi*(R2**2-R1**2)
! cdf = C(r) = (r**2-R1**2)/(R2**2-R1**2)
! pdf = f(phi) = 1/(2*pi)
! cdf = C(phi) = phi/(2*pi)
! M. Ragheb
```



```

program ring_source
! Variables declaration
  real :: radius2 = 1.0
  real :: radius1 = 0.5
  real :: pi = 3.14159
  integer :: trials = 500
  real r, phi, x, y
! Open output file
  open(44, file = 'random_out')
  r1=radius1*radius1
  r2=radius2*radius2
  dr=r2-r1
! Begin sampling points
  do i= 1, trials
! Sample radius on disk
    call random(rr)
    r= sqrt (r1+dr*rr)
! Sample azimuthal angle
    call random(rr)
    phi = 2.0*pi*rr
! Calculate x and y coordinates
    x = r * cos (phi)
    y = r * sin (phi)
! Write sampled points to output file
    write (44,100) x, y
    write(*,*) x, y
100    format (2e14.8)
  end do
end

```

Figure 12. Procedure for sampling a uniform ring source.

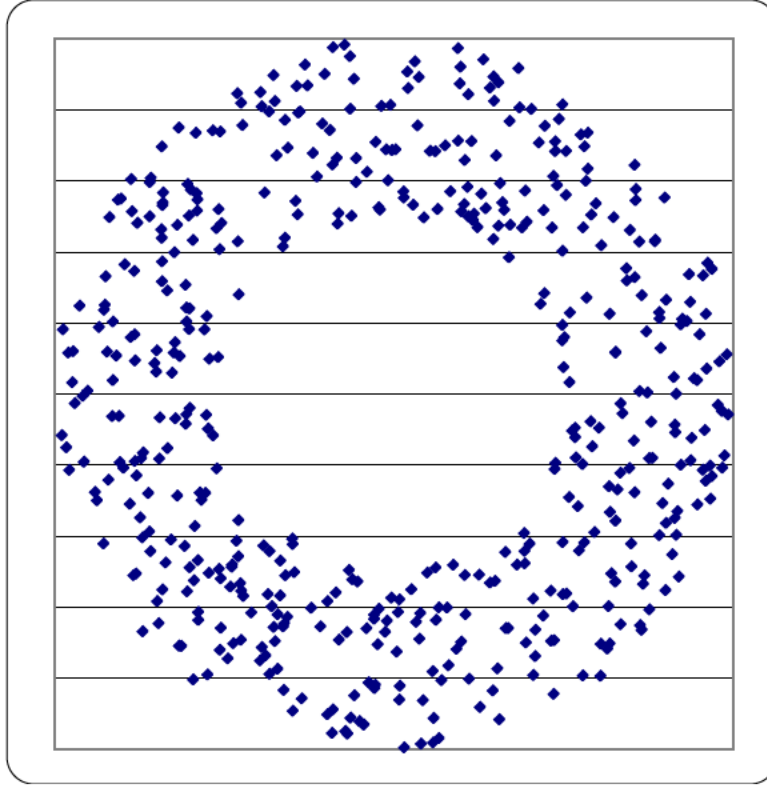


Figure 13. Sampled points of a uniform ring source.

8. SAMPLING A CYLINDRICAL SOURCE

The procedure to sample points uniformly distributed over the volume of a cylindrical source such a fuel element in a nuclear reactor, a spent fuel casket, or the reactor core itself, is a combination of the sampling of the line source and the disk source. In this case the cylindrical probability density function is:

$$\begin{aligned}
 pdf : p(r, \theta, z) dr d\theta dz &= \frac{rd\theta dz dr}{\int_0^R \int_0^H \int_0^{2\pi} rd\theta dz dr} \\
 &= \frac{rdr}{\int_0^R r dr} \cdot \frac{dz}{\int_0^H dz} \cdot \frac{d\theta}{\int_0^{2\pi} d\theta}
 \end{aligned} \tag{32}$$

yields sampled points uniformly distributed over the cylinder volume using three pseudo-random numbers as:

$$\begin{aligned}
 r &= R\rho_1^{1/2} \\
 \theta &= 2\pi\rho_2 \\
 x &= r \cos \theta \\
 y &= r \sin \theta \\
 z &= H\rho_3
 \end{aligned}
 \tag{33}$$

```

! cylinder_source f90
! Sampling sources uniformly distributed in a cylinder of radius R
! and height H
! pdf = f(r) = 2*r/R**2      cdf = C(r) = r**2/R**2
! pdf = f(phi) = 1/(2*pi)    cdf   = C(phi) = phi/(2*pi)
! pdf = f(z) = 1/H          cdf = C(z) = z/H
! M. Ragheb
! program cylinder_source
! Variables declaration
real :: radius = 1.0
real :: height = 1.0
real :: pi = 3.14159
integer :: trials = 1000
real r, phi, x, y, z
! Open output file
open(44, file = 'random_out')
! Begin sampling points
do i= 1, trials
! Sample radius on disk
    call random(rr)
    r= radius * sqrt (rr)
! Alternate radius sampling
! r= radius * rr
! Sample azimuthal angle
    call random(rr)
    phi = 2.0*pi*rr
! Sample height
    call random(rr)
    z= height * rr
! Calculate x and y coordinates
    x = r * cos (phi)
    y = r * sin (phi)
! Write sampled points to output file
    write (44,100) x, y, z
    write(*,*) x, y, z
100    format (3e14.8)
end do
end

```

Figure 14. Procedure for sampling a cylindrical source.

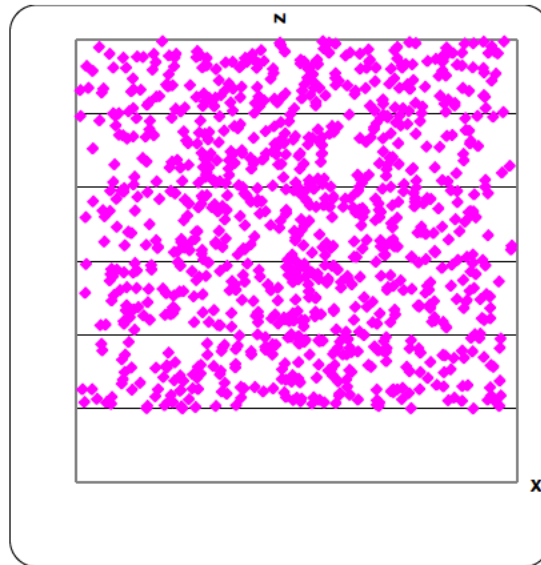


Figure 15. Sampled points for a uniform cylindrical source. $N=1,000$.

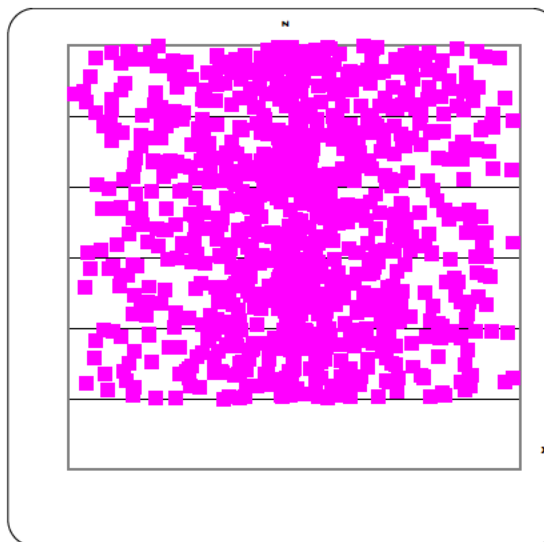


Figure 16. Sampled points for a nonuniform cylindrical source. $N=1,000$.

Figure 14 shows a procedure for sampling a cylindrical source. The uniform source sampled with 1,000 points is shown in Fig. 15. If one had chosen the source as proportional to the pseudo random number rather than its square root, a nonuniform source would have ensued instead of the intended uniform source as shown in Fig. 16.

9. SAMPLING A SPHERICAL SOURCE

For a sphere of radius R we can write for the pdf and cdf in the radial direction:

$$pdf : f(r)dr = \frac{dV}{\int dV} = \frac{4\pi r^2 dr}{\int_0^R 4\pi r^2 dr} = \frac{4\pi r^2 dr}{\frac{4}{3}\pi R^3} \quad (34)$$

$$cdf : C(r) = \frac{\int_0^r 4\pi r^2 dr}{\frac{4}{3}\pi R^3} = \frac{\frac{4}{3}\pi r^3}{\frac{4}{3}\pi R^3} = \rho_1 \quad (35)$$

Inverting the cdf yields for the sampled radius r :

$$r = R\rho_1^{1/3} \quad (36)$$

Notice the different exponent in the case of the spherical case (1/3) compared with the case of the cylindrical geometry (1/2).

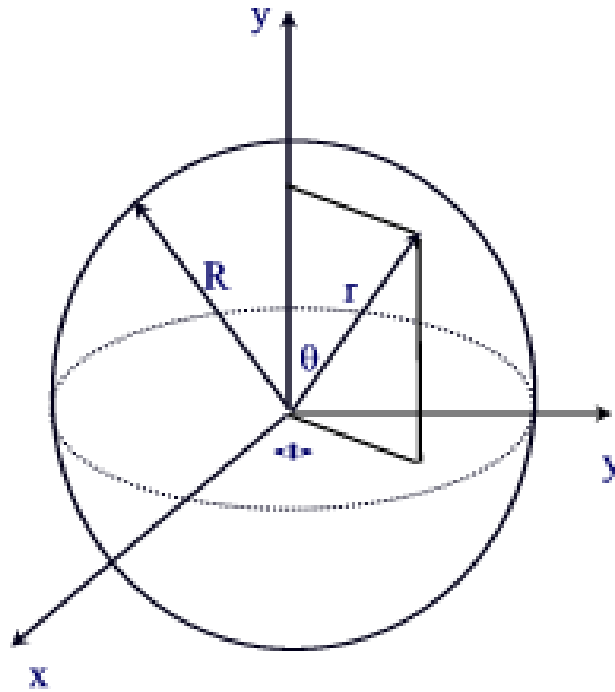


Figure 17. Spherical source geometry.

For the polar angle θ and the azimuthal angle ϕ , we adopt the approach of sampling an isotropic spherically symmetrical source. In this case each element of solid angle receives the same contribution from the source. Hence we need to sample the pdf:

$$\begin{aligned} p(\theta, \phi)d\theta d\phi &= \frac{d\Omega}{4\pi} = \frac{1}{4\pi} \frac{dS}{r^2} = \frac{rd\theta \cdot r \sin \theta d\phi}{4\pi r^2} \\ &= p(\theta) \cdot p(\phi) = \frac{\sin \theta d\theta}{2} \cdot \frac{d\phi}{2\pi} \end{aligned}$$

For the polar angle:

$$pdf : f(\theta)d\theta = \frac{\sin \theta d\theta}{2}, \int_0^\pi \frac{\sin \theta}{2} d\theta = 1$$

$$\begin{aligned} cdf : C(\theta) &= \int_0^\theta \frac{\sin \theta}{2} d\theta \\ &= \frac{1 - \cos \theta}{2} = \rho_2 \\ \mu &= \cos \theta = (1 - 2\rho_2) \\ \theta &= \cos^{-1}(1 - 2\rho_2) \end{aligned}$$

For the azimuthal angle:

$$pdf : f(\phi)d\phi = \frac{d\phi}{2\pi} = \frac{d\phi}{2\pi}$$

$$\begin{aligned} cdf : C(\phi) &= \int_0^\phi \frac{d\phi}{2\pi} = \frac{\phi}{2\pi} = \rho_3 \\ \phi &= 2\pi\rho_3 \end{aligned}$$

Thus the sampled coordinate points in a uniform spherical source would be:

$$\begin{aligned} x &= r \sin \theta \cos \phi = R\rho_1^{1/3} (1 - \mu^2)^{1/2} \cos(2\pi\rho_3) \\ y &= r \sin \theta \sin \phi = R\rho_1^{1/3} (1 - \mu^2)^{1/2} \sin(2\pi\rho_3) \\ z &= r \cos \theta = R\rho_1^{1/3} \mu, \\ \text{where : } \mu &= (1 - 2\rho_2) \end{aligned} \tag{37}$$

Since:

$$\begin{aligned}\cos^2 \theta + \sin^2 \theta &= \mu^2 + \sin^2 \theta = 1 \\ \sin \theta &= (1 - \mu^2)^{1/2}\end{aligned}$$

10. SAMPLING A HEMISPHERICAL SOURCE

This is a special case of the spherical source where the polar angle is as shown in Fig. 18:

$$\theta \in [0, \frac{\pi}{2}].$$

Thus:

$$pdf : f(\theta)d\theta = \sin \theta, \int_0^{\pi/2} \sin \theta d\theta = 1$$

Since:

$$\begin{aligned}p(\theta, \phi)d\theta d\phi &= \frac{d\Omega}{2\pi} = \frac{1}{2\pi} \frac{dS}{r^2} = \frac{rd\theta \cdot r \sin \theta d\phi}{2\pi r^2} \\ &= p(\theta)d\theta \cdot p(\phi)d\phi = \sin \theta d\theta \cdot \frac{d\phi}{2\pi}\end{aligned}$$

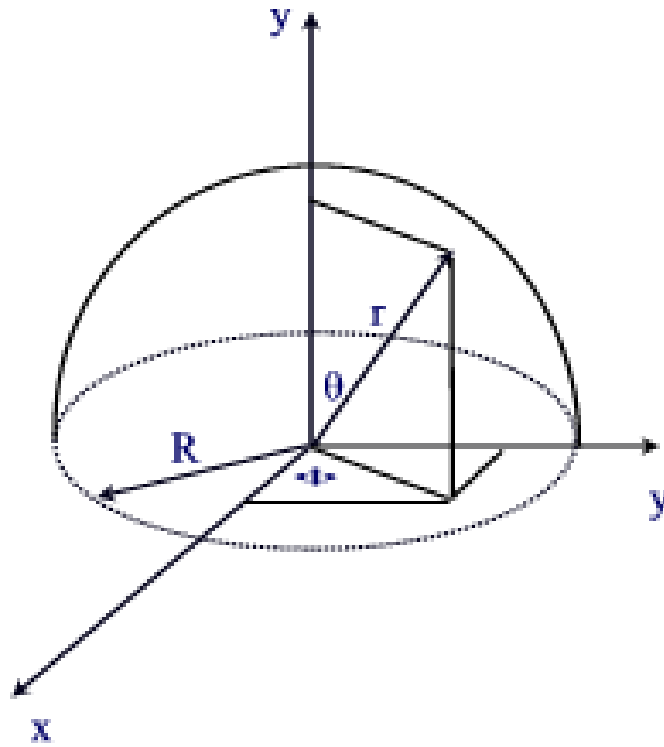


Figure 18. Hemispherical source geometry.

The cdf is:

$$\begin{aligned}
 \text{cdf} : C(\theta) &= \int_0^\theta \sin \theta d\theta \\
 &= 1 - \cos \theta = \rho_2 \\
 \mu &= \cos \theta = (1 - \rho_2) \approx \rho_2 \\
 \theta &= \cos^{-1}(1 - \rho_2) \approx \cos^{-1} \rho_2
 \end{aligned} \tag{38}$$

since $(1 - \rho_2)$ is distributed in the same manner as ρ_2 .

The sampling for the azimuthal angle proceeds in the same way as for the spherical source.

11. SAMPLING A SPHERICAL SHELL

The pdf and cdf for the radial position are in this case:

$$pdf : f(r)dr = \frac{dV}{\int_{R_1}^{R_2} 4\pi r^2 dr} = \frac{4\pi r^2 dr}{\frac{4}{3}\pi(R_2^3 - R_1^3)}$$

$$cdf : C(r) = \frac{\int_{R_1}^r 4\pi r^2 dr}{\frac{4}{3}\pi(R_2^3 - R_1^3)} = \frac{\frac{4}{3}\pi(r^3 - R_1^3)}{\frac{4}{3}\pi(R_2^3 - R_1^3)} = \rho_1 \quad (39)$$

$$r = [R_1^3 + (R_2^3 - R_1^3)\rho_1]^{\frac{1}{3}}$$

The sampling of the polar and azimuthal angles is similar to the case of the hemisphere, yielding the sample points:

$$x = r \sin \theta \cos \phi = [R_1^3 + (R_2^3 - R_1^3)\rho_1]^{\frac{1}{3}} (1 - \mu^2)^{\frac{1}{2}} \cos(2\pi\rho_3)$$

$$y = r \sin \theta \sin \phi = [R_1^3 + (R_2^3 - R_1^3)\rho_1]^{\frac{1}{3}} (1 - \mu^2)^{\frac{1}{2}} \sin(2\pi\rho_3) \quad (40)$$

$$z = r \cos \theta = [R_1^3 + (R_2^3 - R_1^3)\rho_1]^{\frac{1}{3}} \mu,$$

where : $\mu = (1 - 2\rho_2)$

12. SAMPLING A HEMISPHERICAL SHELL

This is a special case of the spherical shell as shown in Fig. 19 where:

$$f(\theta)d\theta = \sin \theta d\theta$$

$$C(\theta) = \int_0^\theta \sin \theta d\theta$$

$$= 1 - \cos \theta = \rho_2$$

$$\mu = \cos \theta = (1 - \rho_2) \approx \rho_2$$

And the sampled points become:

$$\begin{aligned}
 x &= \left[R_1^3 + (R_2^3 - R_1^3) \rho_1 \right]^{1/3} (1 - \mu^2)^{1/2} \cos(2\pi\rho_3) \\
 y &= \left[R_1^3 + (R_2^3 - R_1^3) \rho_1 \right]^{1/3} (1 - \mu^2)^{1/2} \sin(2\pi\rho_3) \\
 z &= \left[R_1^3 + (R_2^3 - R_1^3) \rho_1 \right]^{1/3} \mu
 \end{aligned}
 \tag{41}$$

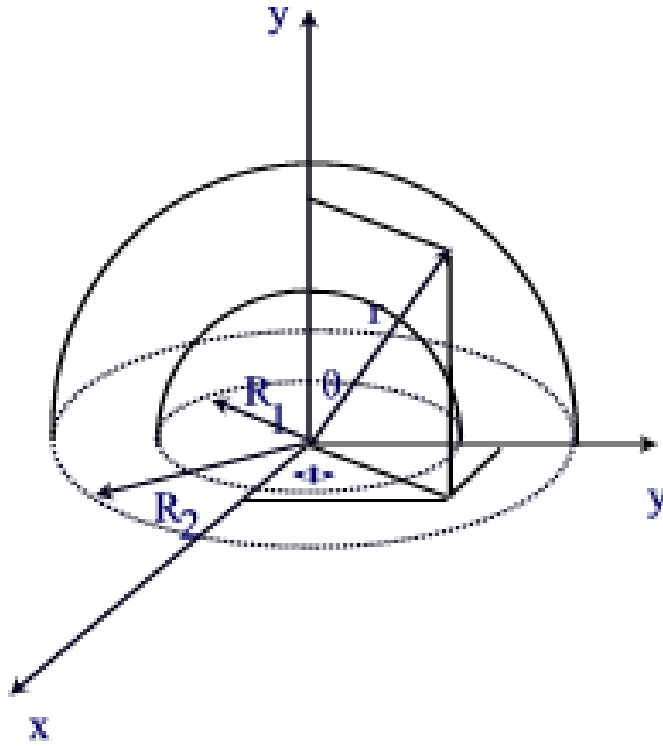


Figure 19. Sampling a hemispherical shell geometry.

13. SAMPLING NON-UNIFORM SOURCES

In most situations one encounters cases where the source distribution is not uniform. For instance the permeability in a porous medium, the conductivity in a conductor or the space charge in a plasma may depend on the coordinates, and would be nonuniform. In flow problems, in particular, one encounters the need to set a random radius in a uniform axisymmetric flow. As an example we consider a spherical source

case with a variate such as the probability of a radius r is proportional to r . A volumetric density of source particles describing this situation is given by:

$$f(r) = kr \quad (42)$$

where k is a constant.

The pdf in this case is modified from Eqn. 35 as:

$$\begin{aligned} pdf : f(r)dr &= \frac{4\pi r^2 f(r)dr}{\int_0^R 4\pi r^2 f(r)dr} = \frac{4\pi r^2 (kr)dr}{\int_0^R 4\pi r^2 (kr)dr} \\ &= \frac{4\pi kr^3 dr}{\int_0^R 4\pi kr^3 dr} = \frac{4\pi r^3 dr}{\pi R^4} \end{aligned} \quad (43)$$

and the cdf is:

$$cdf : C(r) = \frac{\int_0^r 4\pi r^3 dr}{\pi R^4} = \frac{\pi r^4}{\pi R^4} = \rho \quad (44)$$

Thus the sampled radius is given by:

$$r = R\rho^{1/4} \quad (45)$$

The polar and azimuthal angles can be sampled in a way similar to the case for a uniform spherical source.

14. SAMPLING DISTRIBUTIONS WHICH ARE NOT PROBABILITY DENSITY FUNCTIONS

Consider a random variable that is defined over the interval:

$$\xi \in [3, 5]$$

that is distributed proportional to x^3 in this region. The function x^3 can be converted to a probability density function with proper normalization. In this case the pdf is:

$$f(x)dx = \frac{x^3 dx}{\int_3^5 x^3 dx} = \frac{x^3 dx}{[x^4/4]_3^5} = \frac{x^3 dx}{\frac{(5^4 - 3^4)}{4}}$$

The cumulative distribution function is constructed and equated to pseudo random number ρ :

$$C(x) = \frac{\int_3^x x^3 dx}{\int_3^5 x^3 dx} = \frac{\frac{1}{4}(x^4 - 3^4)}{\frac{(5^4 - 3^4)}{4}} = \frac{(x^4 - 3^4)}{(5^4 - 3^4)} = \rho$$

Inverting the cdf, we get the sampling function:

$$x = [3^4 + (5^4 - 3^4)\rho]^{1/4}. \quad (46)$$

15. SURFACE SOURCE EMITTING A COSINE DISTRIBUTION

This situation occurs in dosimetry and shielding studies as well as in fluid dynamics when a particle reservoir is used as a boundary condition. For a total surface source strength S_0 [particles/(cm².sec)], the source differential angular distribution is given by:

$$S(\theta) = S_0 \frac{\cos \theta}{2\pi} \left[\frac{\text{particles}}{\text{sec.cm}^2 \cdot \text{steradian}} \right] \quad (47)$$

since:

$$d\Omega = \frac{dS}{r^2} = \frac{r^2 \sin \theta d\theta d\phi}{r^2} = \sin \theta d\theta d\phi$$

The un-normalized pdf for sampling such a source is given by:

$$\begin{aligned} p(\theta, \phi) d\theta d\phi &= S(\theta) \cdot d\Omega \\ &= \frac{S_0 \cos \theta}{2\pi} \cdot d\Omega \\ &= \frac{S_0 \cos \theta}{2\pi} \cdot \sin \theta d\theta d\phi \\ &= f(\theta) d\theta \cdot f(\phi) d\phi \\ &= S_0 \sin \theta \cos \theta d\theta \cdot \frac{d\phi}{2\pi} \end{aligned}$$

The pdf for the polar angle needs to be normalized as discussed in the last section:

$$\begin{aligned}
pdf : f(\theta)d\theta &= \frac{S_0 \sin \theta \cos \theta d\theta}{S_0 \int_0^{\pi/2} \sin \theta \cos \theta d\theta} \\
&= \frac{-\cos \theta d(\cos \theta)}{-\int_0^{\pi/2} \cos \theta d(\cos \theta)} \\
&= \frac{2 \cos \theta d(\cos \theta)}{[\cos^2 \theta]_0^{\pi/2}} \\
&= -2 \cos \theta d(\cos \theta)
\end{aligned}$$

The cdf becomes:

$$\begin{aligned}
cdf : C(\theta) &= -\int_0^{\theta} 2 \cos \theta d(\cos \theta) \\
&= \int_{\theta}^0 2 \cos \theta d(\cos \theta) \\
&= 1 - \cos^2 \theta = \rho
\end{aligned}$$

Inverting the cdf:

$$\begin{aligned}
\cos^2 \theta &= 1 - \rho \approx \rho \\
\cos \theta &= \rho^{1/2} \\
\theta &= \cos^{-1}(\rho^{1/2})
\end{aligned} \tag{48}$$

16. SAMPLING SPATIAL DISTRIBUTIONS

We consider the case of sampling the flux or power distribution in a rectangular parallelepiped reactor core with side lengths a , b , and c in the x , y , and z directions respectively, as shown in Fig. 20. Sampling the neutron flux may be needed for shielding calculations.

The neutron source is proportional to the flux distribution:

$$\phi(x, y, z) = \phi_0 \cos\left(\frac{\pi x}{a}\right) \cos\left(\frac{\pi y}{b}\right) \cos\left(\frac{\pi z}{c}\right) \tag{49}$$

If one would sample a uniform source distribution the corresponding pdf would be:

$$\begin{aligned}
 f(x, y, z)dxdydz &= \int dV \\
 &= \frac{dxdydz}{\int_{-a/2}^{+a/2} dx \int_{-b/2}^{+b/2} dy \int_{-c/2}^{+c/2} dz} \\
 &= \frac{dxdydz}{abc}
 \end{aligned}$$

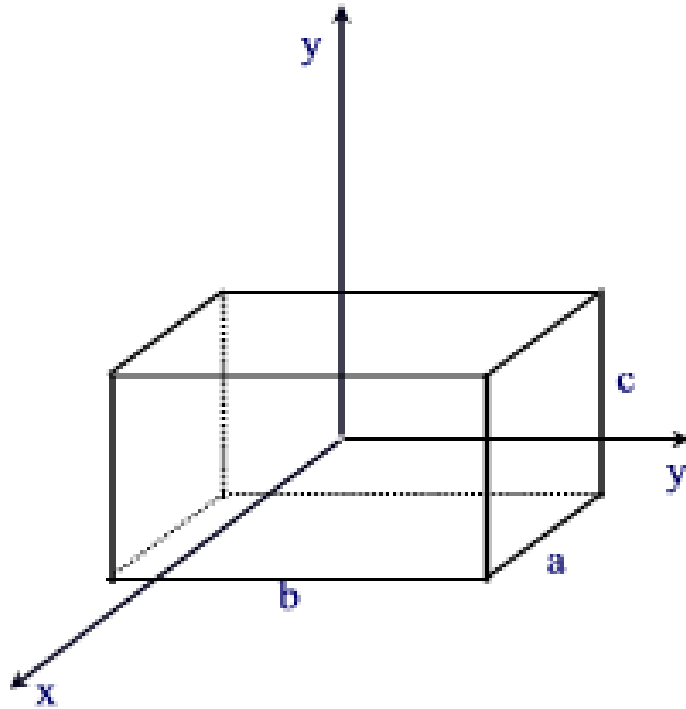


Figure 20. Flux distribution in a rectangular parallelepiped reactor.

This is separable in the x, y, and z directions as follows:

$$\begin{aligned}
 f(x, y, z)dxdydz &= f(x)dx.f(y)dy.f(z)dz \\
 &= \frac{dx}{a} \frac{dy}{b} \frac{dz}{c}
 \end{aligned}$$

The corresponding cdfs and sampled points become:

$$\begin{aligned}
 C(x) &= \frac{\int_{-a/2}^x dx}{a} = \frac{x + \frac{a}{2}}{a} = \rho_1 \Rightarrow x = a\rho_1 - \frac{a}{2} \\
 C(y) &= \frac{\int_{-b/2}^y dy}{b} = \frac{y + \frac{b}{2}}{b} = \rho_2 \Rightarrow y = b\rho_2 - \frac{b}{2} \\
 C(z) &= \frac{\int_{-c/2}^z dz}{c} = \frac{z + \frac{c}{2}}{c} = \rho_3 \Rightarrow z = c\rho_3 - \frac{c}{2}
 \end{aligned} \tag{50}$$

This result can be generalized if the flux distribution of Eqn. 49 is considered. In this case the pdf can be written as:

$$\begin{aligned}
 f(x, y, z)dxdydz &= \frac{\phi(x, y, z)dV}{\int \phi(x, y, z)dV} \\
 &= \frac{\phi_0 \cos\left(\frac{\pi x}{a}\right) \cos\left(\frac{\pi y}{b}\right) \cos\left(\frac{\pi z}{c}\right) dx dy dz}{\phi_0 \int_{-a/2}^{+a/2} \cos\left(\frac{\pi x}{a}\right) dx \int_{-b/2}^{+b/2} \cos\left(\frac{\pi y}{b}\right) dy \int_{-c/2}^{+c/2} \cos\left(\frac{\pi z}{c}\right) dz}
 \end{aligned}$$

Since:

$$\int_{-a/2}^{+a/2} \cos \frac{\pi x}{a} dx = \frac{a}{\pi} \left[\sin \frac{\pi x}{a} \right]_{-a/2}^{+a/2} = \frac{2a}{\pi}$$

we can write:

$$\begin{aligned}
 f(x, y, z)dxdydz &= f(x)dx \cdot f(y)dy \cdot f(z)dz \\
 &= \frac{\pi}{2a} \cos\left(\frac{\pi x}{a}\right) dx \cdot \frac{\pi}{2b} \cos\left(\frac{\pi y}{b}\right) dy \cdot \frac{\pi}{2c} \cos\left(\frac{\pi z}{c}\right) dz
 \end{aligned}$$

The corresponding cdfs are:

$$C(x) = \frac{\pi}{2a} \int_{-a/2}^x \cos\left(\frac{\pi x}{a}\right) dx = \frac{1}{2} \left[\sin\left(\frac{\pi x}{a}\right) + 1 \right] = \rho_1$$

$$C(y) = \frac{\pi}{2b} \int_{-b/2}^y \cos\left(\frac{\pi y}{b}\right) dy = \frac{1}{2} \left[\sin\left(\frac{\pi y}{b}\right) + 1 \right] = \rho_2$$

$$C(z) = \frac{\pi}{2c} \int_{-c/2}^z \cos\left(\frac{\pi z}{c}\right) dz = \frac{1}{2} \left[\sin\left(\frac{\pi z}{c}\right) + 1 \right] = \rho_3$$

The sampled points representing the neutron source distribution will be:

$$\begin{aligned} x &= \frac{a}{\pi} \sin^{-1}(2\rho_1 - 1) \\ y &= \frac{b}{\pi} \sin^{-1}(2\rho_2 - 1) \\ z &= \frac{c}{\pi} \sin^{-1}(2\rho_3 - 1) \end{aligned} \quad (51)$$

EXERCISES

1. Write a procedure to sample the Maxwell-Boltzmann distribution for velocities and the distribution for energies at room temperature. Make sure that the form you use is normalized. Graphically estimate the most probable energy and velocity, as well as the average velocity and energy.
2. Write a procedure to simulate the process of radioactive decay of a radioactive isotope with decay constant λ , whose probability density function is:

$$\begin{aligned} pdf : p(t) &= \lambda e^{-\lambda t} \\ \lambda &= \frac{\ln 2}{T_{1/2}} = \frac{0.6931}{T_{1/2}} \end{aligned}$$

where: $T_{1/2}$ is the half life of the isotope.

Simulate the decay of tritium whose half-life is 12.34 [years], and display the frequency distribution that the procedure generates.

3. In the sampling procedure for the Normal distribution based upon the Central Limit Theorem, the number of uniformly distributed random variables is taken as 12. Investigate the effect on the generated distribution if a smaller number, say 5 is used, or a larger number, say 20 is used.
4. Modify the procedure to sample a uniform cylindrical source to sample a cylindrical shell of height h , and radii R_1 and R_2 .
5. Derive the probability density function, the cumulative distribution function and the sampling procedure to sample an isotropic radiation source:
 - a) In the upper positive hemisphere,

b) In the upper positive quadrant.