CHAPTER

21

Introduction to Monte Carlo Methods

OUTLINE

"Everything is composed of small particles of itself and they are flying around in concentric circles and arcs and segments and innumerable other geometrical figures too numerous to mention collectively, never standing still or resting but spinning away and darting hither and thither and back again, all the time on the go. These diminutive gentlemen are called atoms. Do you follow me intelligently?"

–*Flann O'Brien,* The Third Policeman

CHAPTER POINTS

- Monte Carlo methods give us a way to simulate the behavior of radiation without having to resort to discretized differential equations.
- Using sampling and tracking of individual, simulated neutrons we can solve shielding problems using realistic materials.
- Rejection sampling is a technique for drawing random numbers from a distribution where we do not know the cumulative density function.

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21.1 ANALOG PHYSICS

In this chapter we will use Python to create synthetic neutrons. We will then follow these neutrons to see what will happen in a system. The process of using simulated, synthetic particles that behave in a similar manner as actual neutrons (or other particles) is an example of analog physics. This gives a retro-sounding ring to the process, like it is something that goes along with vinyl records and vacuum-tube amplifiers. We mean here that our synthetic neutrons are analogs of true neutrons.

The way we will deal with these particles is using random sampling of their interactions, just as quantum mechanics governs the behavior of particles using probabilities. This is different than what we did in diffusion methods for simulating neutron behavior: in those models we derived differential equations for the expected behavior of a collection of neutrons. In analog physics we simulate many particles and then we compute the mean behavior (or other quantities that interest us).

These methods are called Monte Carlo methods. The first modern Monte Carlo methods were developed by Stanislaw Ulam during the Manhattan Project, and Nicholas Metropolis coined the name after a famous casino. One benefit of Monte Carlo methods is that they require much less mathematics in the algorithms. Once we know how to draw random numbers appropriately, we just need to "roll dice" many, many times to get the answer.

21.2 PROBABILITY PRELIMINARIES

We will need to know a few things about probabilities before we begin. A cumulative distribution function (CDF) is defined as a function $F(x)$ that is the probability that a random variable c, from a particular distribution, is less than x. In mathematical form we write this as

$$F(x) = P(c < x).$$

Because probabilities are always in the range [0, 1], the function $F(x) \in [0, 1]$. As an example, consider the random variable defined by the value of a roll of a single die. In this case, the CDF is given by

$$F(x) = \begin{cases} 0 & x \leq 1 \\ \frac{1}{6} & 1 < x \leq 2 \\ \frac{1}{3} & 2 < x \leq 3 \\ \frac{1}{2} & 3 < x \leq 4 \\ \frac{2}{3} & 4 < x \leq 5 \\ \frac{5}{6} & 5 < x \leq 6 \\ 1 & 6 < x \end{cases}.$$

Using this definition, $F(6.1)$ is 1, because it is certain that the roll will give a number less than 6.1.

The way that the CDF is defined leads to two important limits:

$$\lim_{x\to\infty} F(x) = 1, \qquad \text{and} \qquad \lim_{x\to-\infty} F(x) = 0.$$

Along with the CDF we will use the probability density function (PDF) , written as $f(x)$. The PDF is defined such that

$$f(x)dx = \text{The probability that the random variable is in } dx \text{ about } x.$$

The PDF is the derivative of the CDF and they are related by

$$f(x) = \frac{dF}{dx}, \qquad \text{and} \qquad F(x) = \int_{-\infty}^{x} f(x')\,dx'.$$

Also, from these relations we get

$$\int_{-\infty}^{\infty} f(x)\,dx = 1.$$

This relation shows that probability densities are normalized to 1 and can be interpreted as the probability of the random variable being between $-\infty$ and ∞ is 1.

Going back to the roll of a single die, the PDF for this random variable is the sum of Dirac delta functions because the value of a roll can only be the integers 1–6. This PDF is

$$f(x) = \frac{1}{6}\left[\delta(x-1) + \delta(x-2) + \delta(x-3) + \delta(x-4) + \delta(x-5) + \delta(x-6)\right].$$

Notice that the factor of one-sixth is required to satisfy the normalization condition.

Using the PDF we can find the expected value of some function of the random variable. Consider the function $g(x)$, the expected value of this function, $E[g(x)]$, is defined by the integral

$$E[g(x)] = \int_{-\infty}^{\infty} g(x) f(x)\,dx.$$

An important expected value is the mean of the random variable. The mean is found by determining the expected value of the function $g(x) = x$. The mean is sometimes written as $\bar{x}$ and it is defined as

$$\bar{x} = \int_{-\infty}^{\infty} x f(x)\,dx.$$

21.3 THE EXPONENTIAL DISTRIBUTION

The most important distribution for Monte Carlo methods for neutron transport is the exponential distribution. This is because the probability that a neutron travels a number of mean-free paths in $d\lambda$ about λ before having a collision is given by

$$f(\lambda)\,d\lambda = e^{-\lambda}\,d\lambda, \text{ for } \lambda > 0.$$

This distribution tells us that if N neutrons travel λ mean-free paths without a collision, then we expect Ne^{-1} neutrons to travel $\lambda + 1$ mean-free paths. The average distance traveled by a neutron without having a collision, in units of mean-free paths, based on this distribution can be found via the integral

$$\bar{\lambda} = \int_0^\infty \lambda e^{-\lambda}\,d\lambda = 1.$$

This shows why we call λ the mean-free path: it is the expected distance a neutron will travel without having a collision.

Usually, we want to work in units of distance rather than mean-free paths. To convert the exponential distribution to be a function of distance, rather than mean-free paths, we use the total macroscopic cross-section for the material times a distance to write

$$\Sigma_t x = \lambda, \qquad d\lambda = \Sigma_t dx.$$

Making this substitution we get the PDF for the exponential distribution as

$$f(x) = \Sigma_t e^{-\Sigma_t x}.$$

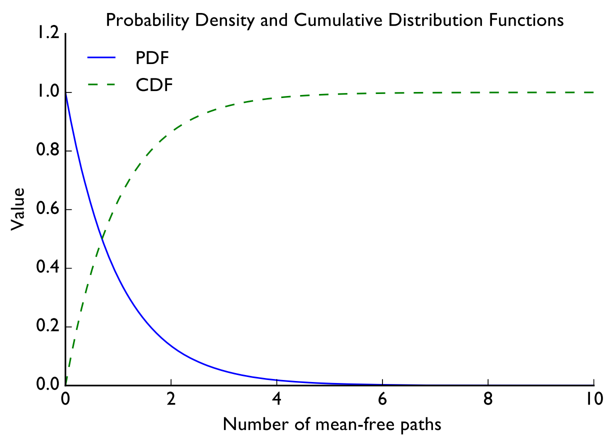
We can check that this is a proper PDF by integrating over all x and seeing that the integral equals one

$$\int_0^\infty dx\,\Sigma_t e^{-\Sigma_t x} = -\,e^{-\Sigma_t x}\Big|_0^\infty = 1.$$

From this we can also define the CDF:

$$F(x) = \int_0^x dx\,\Sigma_t e^{-\Sigma_t x} = -\,e^{-\Sigma_t x}\Big|_0^x = 1 - e^{-\Sigma_t x}.$$

Below is a plot of the CDF and PDF:



21.4 A FIRST MONTE CARLO PROGRAM

Now we would like to use Monte Carlo solve the following problem: a beam of neutrons strikes a 3 cm thick slab of material with $\Sigma_\mathrm{t} = 2.0$ cm^{-1}. What fraction of the neutrons get through the slab without a collision? Using the results from the previous section, we know that the answer to this problem is defined by the integral

$$\int_3^\infty \Sigma_\mathrm{t} e^{-\Sigma_\mathrm{t} x}\,dx = e^{-2\times 3} \approx 0.002478752177.$$

We would like to solve this problem with Monte Carlo using the following procedure

1. Create neutron.
2. Sample randomly a distance to collision from the exponential distribution.
3. Check to see if the distance to collision is greater than 3.
4. Go back to 1 until we've run "enough" neutrons.

At the end of this procedure the ratio of the number of neutrons that went through the slab to those that we created is the fraction that we are looking for.

The hard part is that we do not know how to generate a random sample from the exponential distribution. We do, however, know how to get a random number between 0 and 1 using NumPy's random function or the functions from the `random` module. We also know that the CDF, $F(x)$, is always between 0 and 1. Therefore, the following procedure can give me a random number from the exponential distribution:

1. Pick a random number between 0 and 1, call it θ
2. Invert the CDF to solve for x in $F(x) = \theta$; this value of x is my random sample.

In our case we need to solve for x in

$$\theta = 1 - e^{-\Sigma_\mathrm{t} x},$$

which gives us

$$x = \frac{-\log(1-\theta)}{\Sigma_\mathrm{t}}.$$

We can translate this algorithm to Python in a few short steps. The algorithm will require the user to enter the number of neutrons requested, N, and the thickness of the slab and the macroscopic cross-section for the material.

```
In [2]: def slab_transmission(Sig_t,thickness,N):
            """Compute the fraction of neutrons that leak through a slab
            Inputs:
            Sig_t:     The total macroscopic x-section
            thickness: Width of the slab
            N:         Number of neutrons to simulate

            Returns:
            transmission:  The fraction of neutrons that made it through
```

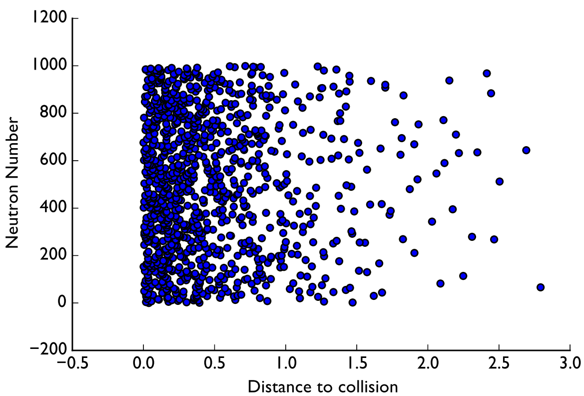
```
    """
    thetas = np.random.random(N)
    x = -np.log(1-thetas)/Sig_t
    transmission = np.sum(x>thickness)/N

    #for a small number of neutrons we'll output a little more
    if (N<=1000):
        plt.scatter(x,np.arange(N))
        plt.xlabel("Distance to collision")
        plt.ylabel("Neutron Number")
    return transmission
```

BOX 21.1 PYTHON PRINCIPLE

NumPy can generate random numbers from a variety of distributions. The most common two we use for Monte Carlo simulations are `np.random.random(N)`, which gives `N` random numbers between 0 and 1, and `np.random.uniform(lower, upper, N)`, which gives `N` random numbers between `lower` and `upper`. For both of these there are single-value versions in the `random` library: `random.random()` and `random.uniform(lower, upper)`. In the `np.random` and `random` libraries there are more exotic distributions built-in as well.

To test this function we will execute it with a small number of neutrons and look at where the collisions take place. The function will make a graph showing where neutrons had a collision if the number of neutrons is less than or equal to 1000. This initial run will use 1000 neutrons to test this feature.

```
In [3]: #test the functionwith a small number of neutrons
        Sigma_t = 2.0
        thickness = 3.0
        N = 1000
        transmission = slab_transmission(Sigma_t, thickness, N)
        print("Out of",N,"neutrons only",int(transmission*N),
              "made it through.\n The fraction that made it through was",
              transmission)
```



```
Out of 1000 neutrons only 4 made it through.
 The fraction that made it through was 0.004
```

Notice that most of the neutrons have a collision very close to the edge of the slab. Only 4 out of 1000 made it all the way through the slab (that is, only 4 had a distance to collision greater than 3). In this case we get a pretty good answer to our question (0.004 is off by less than a factor of two), but we can check that it converges to the correct answer as $N \to \infty$.

```
In [4]:  neuts = np.array([2000,4000,8000,16000,32000,
                           64000,128000,256e3,512e3,1024e3,2056e3])
         for N in neuts:
             transmission = slab_transmission(Sigma_t, thickness, N)
             print("Out of",N,"neutrons only",int(transmission*N),
                   "made it through.\n The fraction that made it through was",
                   transmission)
```

```
Out of 2000.0 neutrons only 6 made it through.
 The fraction that made it through was 0.003
Out of 4000.0 neutrons only 13 made it through.
 The fraction that made it through was 0.00325
Out of 8000.0 neutrons only 29 made it through.
 The fraction that made it through was 0.003625
Out of 16000.0 neutrons only 47 made it through.
 The fraction that made it through was 0.0029375
Out of 32000.0 neutrons only 73 made it through.
 The fraction that made it through was 0.00228125
Out of 64000.0 neutrons only 165 made it through.
 The fraction that made it through was 0.002578125
Out of 128000.0 neutrons only 341 made it through.
 The fraction that made it through was 0.0026640625
Out of 256000.0 neutrons only 618 made it through.
 The fraction that made it through was 0.0024140625
Out of 512000.0 neutrons only 1285 made it through.
 The fraction that made it through was 0.002509765625
Out of 1024000.0 neutrons only 2528 made it through.
 The fraction that made it through was 0.00246875
Out of 2056000.0 neutrons only 5176 made it through.
 The fraction that made it through was 0.00251750972763
```

We need about 1 million simulated neutrons to get to two digits of the correct answer. Also, if we ran this again we would get different answers because we are using random numbers. The run-to-run variability in the answers is often quantified using the standard deviation. This variability can be thought of as the error in the Monte Carlo calculation. Practitioners often call this variability noise. The error will go down slowly because the way that Monte Carlo works. The standard deviation of the estimate when we look at the run-to-run variability will decrease at a rate proportional to $1/\sqrt{N}$. This means that to cut the error in half we need to quadruple the number of neutrons. Another way to think about it is to say that Monte Carlo methods are one-half order accurate. The $1/\sqrt{N}$ convergence is valid for large values of N and is a result of the central limit theorem.

BOX 21.2 NUMERICAL PRINCIPLE

Running a Monte Carlo calculation multiple times, even with the same number of neutrons, will give you different answers. The standard deviation of this variability is proportional to $N^{-\frac{1}{2}}$, where N is the number of neutrons used in the calculation. This variability manifests itself as errors in the solution and, therefore, we want the standard deviation to be small. The standard deviation goes to zero slowly as $N \to \infty$: to cut the standard deviation in half, one needs to quadruple the number of neutrons.

21.5 ISOTROPIC NEUTRONS ON A SLAB

Even though it takes a lot of particles to make the error in Monte Carlo small, that does not mean it is a bad method. In fact, the nice thing about Monte Carlo is that you have to know very little about the mathematics of the system, all you have to do is be able to push particles around and roll dice. To demonstrate this we will make our problem a little harder. Now say that the neutrons hitting the slab are not a beam but a distribution of neutrons where a neutron's path of flight relative to the normal direction to the slab is measured by the angle ϕ. We say that the distribution of neutrons in angle relative to the slab is uniform in the cosine of the angle ϕ, i.e., the neutrons are isotropic in the cosine of the angle. The angles $\phi \in [-\pi/2, \pi/2]$ point into the slab, this means that the quantity $\cos\phi$ is uniformly distributed between 0 and 1.

For a neutron traveling in direction ϕ the slab can look thicker than 3.0 cm, because if the neutron is traveling at a grazing angle to the slab it will have to travel through more of the slab to get to the other side. We can express this as

$$\text{thickness}(\phi) = \frac{3}{\cos\phi}.$$

A quick check reveals that this gives us what we want: when $\phi = 0$ the neutron is traveling straight through the slab and the thickness to that neutron is 3 cm. Also, when $\phi = \pm\pi/2$ the thickness of the slab is infinite because the neutron is traveling parallel to the slab.

We can make the math easier by defining $\mu = \cos\phi$ and noticing that $\mu \in [0, 1]$. To handle our more complicated problem we make a small change to our Monte Carlo method to have each neutron have its own angle of flight relative to the slab.

1. Create neutron with μ sampled from the uniform distribution $\mu \in [0, 1]$.
2. Sample randomly a distance to collision from the exponential distribution.
3. Check to see if the distance to collision is greater than $3/\mu$.
4. Go back to 1 until we have run "enough" neutrons.

The only change is that now we pick μ uniformly between 0 and 1 (recall that each value of the cosine of the angle was equally likely. That is why this is a random distribution). Furthermore, we check to see if the distance to collision is greater than $3/\mu$. Those are the only changes.

The solution to this problem is more complicated to find mathematically, but the answer is expressed by the exponential integral function:

$$\text{transmission} = \int_0^1 \frac{d\mu}{\Sigma_\mathrm{t}}\, e^{-\Sigma_\mathrm{t} x/\mu} = E_2(\Sigma_\mathrm{t} x).$$

For our case of $x = 3.0$ and $\Sigma_\mathrm{t} = 2$ we get

$$E_2(6) \approx 0.000318257.$$

Notice how the transmission went down because most particles will not have $\mu = 1$.

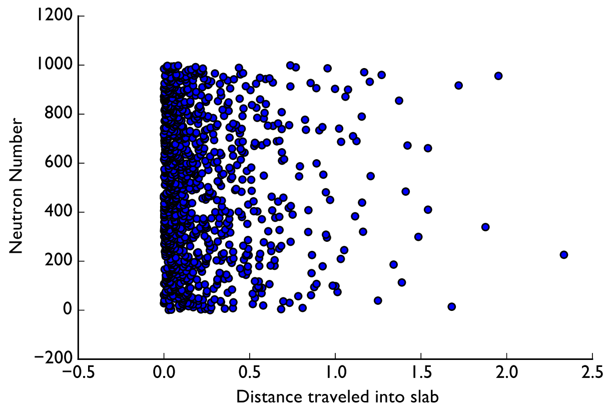
We can simply modify our function above to handle this case. We do this by modifying the previous function to take as an input parameter whether the neutrons are isotropic in the cosine of the incident angle.

```
In [5]: def slab_transmission(Sig_t,thickness,N,isotropic=False):
            """Compute the fraction of neutrons that leak through a slab
            Inputs:
            Sig_t:     The total macroscopic x-section
            thickness: Width of the slab
            N:         Number of neutrons to simulate
            isotropic: Are the neutrons isotropic or a beam

            Returns:
            transmission:  The fraction of neutrons that made it through
            """
            if (isotropic):
                mu = np.random.random(N)
            else:
                mu = np.ones(N)
            thetas = np.random.random(N)
            x = -np.log(1-thetas)/Sig_t
            transmission = np.sum(x>thickness/mu)/N

            #for a small number of neutrons we'll output a little more
            if (N<=1000):
                plt.scatter(x*mu,np.arange(N))
                plt.xlabel("Distance traveled into slab")
                plt.ylabel("Neutron Number")
            return transmission
```

As before we will run the algorithm with a small number of neutrons and visualize where the interactions take place. The figure will now show the distance the neutron travels before a collision as measured from the face the of slab.

```
In [6]: ###testthe function with a small number of neutrons
        Sigma_t = 2.0
        thickness = 3.0
```

```
N = 1000
transmission = slab_transmission(Sigma_t, thickness, N, isotropic=True)
print("Out of",N,"neutrons only",int(transmission*N),
      "made it through.\n The fraction that made it through was",
      transmission)
```




```
Out of 1000 neutrons only 0 made it through.
 The fraction that made it through was 0.0
```

When the neutrons enter the slab at different angles, fewer transmit through the slab without a collision. In this case, none made it through the slab. Also, notice that the scale of the figure changed because no neutron made it more the 2.5 cm into the slab. We can do the same convergence study as before by increasing the number of simulated neutrons and looking at the accuracy of the calculations.

```
In [7]:  neuts = np.array([2000,4000,8000,16000,32000,
                            64000,128000,256e3,512e3,1024e3,2056e3])
         for N in neuts:
             transmission = slab_transmission(Sigma_t, thickness, N, isotropic=True)
             print("Out of",N,"neutrons only",int(transmission*N),
                   "made it through.\n The fraction that made it through was",
                   transmission)
```

```
Out of 2000.0 neutrons only 0 made it through.
 The fraction that made it through was 0.0
Out of 4000.0 neutrons only 0 made it through.
 The fraction that made it through was 0.0
Out of 8000.0 neutrons only 3 made it through.
 The fraction that made it through was 0.000375
Out of 16000.0 neutrons only 3 made it through.
 The fraction that made it through was 0.0001875
Out of 32000.0 neutrons only 11 made it through.
 The fraction that made it through was 0.00034375
Out of 64000.0 neutrons only 20 made it through.
 The fraction that made it through was 0.0003125
Out of 128000.0 neutrons only 30 made it through.
 The fraction that made it through was 0.000234375
```

```
Out of 256000.0 neutrons only 73 made it through.
 The fraction that made it through was 0.00028515625
Out of 512000.0 neutrons only 140 made it through.
 The fraction that made it through was 0.0002734375
Out of 1024000.0 neutrons only 324 made it through.
 The fraction that made it through was 0.00031640625
Out of 2056000.0 neutrons only 717 made it through.
 The fraction that made it through was 0.00034873540856
```

We do start to get to the correct answer, but since so few neutrons get through we have to simulate a lot of them. Here is the result if we try 10 million:

```
In [8]:  N = 1e7
         transmission = slab_transmission(Sigma_t, thickness, N, isotropic=True)
         print("Out of",N,"neutrons only",int(transmission*N),
               "made it through.\n The fraction that made it through was",
               transmission)

Out of 10000000.0 neutrons only 3164 made it through.
 The fraction that made it through was 0.0003164
```

We are getting several digits of accuracy, but it took a lot of neutrons. Of course in real life 10 million neutrons is not very many. We typically talk about neutrons in numbers like 10^{10} or greater. This is the price to pay with analog physics: the number of our pretend neutrons are always going to be smaller that the actual neutrons.

21.6 A FIRST MONTE CARLO SHIELDING CALCULATION

Both problems that we solved above can be solved pretty easily by hand. To make the problem more difficult we can add some scattering. We want to know what fraction of the neutrons get through the slab before being absorbed. This is a typical question in radiation shielding.

In particular, say that the slab is made up of a material that has $\Sigma_t = 2.0$ cm^{-1}, $\Sigma_s = 0.75$ cm^{-1}, and $\Sigma_a = 1.25$ cm^{-1}. Also, say that the neutrons are scattered isotropically when they scatter, that is the direction can change to any other direction upon scattering. This problem cannot be solved very well by diffusion (remember diffusion is an approximation). We can solve it by modifying our procedure from before.

We will need to add the fact that a collision can be a scatter or an absorption. We will still sample a distance to collision using the exponential distribution and the total macroscopic cross-section, $\Sigma_t = \Sigma_s + \Sigma_a$, as before. The difference is that when the neutron collides, we sample whether it is absorbed or scattered based on the scattering ratio: Σ_s/Σ_t. If it scatters, we sample another μ for it and keep following it. Otherwise, we stop following the neutron because it has been absorbed.

The algorithm for this problem just builds on what we did before.

1. Create a counter, $t = 0$ to track the number of neutrons that get through.
2. Create neutron with μ sampled from the uniform distribution $\mu \in [0, 1]$. Set $x = 0$.

3. Sample randomly a distance to collision, l, from the exponential distribution.
4. Move the particle to $x = x + l\mu$.
5. Check to see if $x > 3$. If so $t = t + 1$. Check if $x < 0$, if so go to 2.
6. Sample a random number s in [0,1], if $s < \Sigma_s/\Sigma_t$, the particle scatters and sample $\mu \in [-1, 1]$ and go to step 3. Otherwise, continue.
7. Go back to 2 until we have run "enough" neutrons.

In this case we need to check to make sure that the neutron does not exit the slab at $x = 0$. This is now possible because a scattered neutron can travel backwards toward the face of the slab. If that happens, to our mind that is the same as absorption because that neutron is not going to transmit through the slab.

Our algorithm is going to have to change a lot in this case. For each created neutron we have to follow it until it leaks out of the slab or is absorbed. This could be many collisions if the scattering ratio is high and Σ_t is large. Nevertheless, we can modify the steps of the simple algorithm to simulate this more complicated scenario.

```
In [9]:  def slab_transmission(Sig_s,Sig_a,thickness,N,isotropic=False):
             """Compute the fraction of neutrons that leak through a slab
             Inputs:
             Sig_s:     The scattering macroscopic x-section
             Sig_a:     The absorption macroscopic x-section
             thickness: Width of the slab
             N:         Number of neutrons to simulate
             isotropic: Are the neutrons isotropic or a beam

             Returns:
             transmission:  The fraction of neutrons that made it through
             """
             Sig_t = Sig_a + Sig_s
             iSig_t = 1/Sig_t
             transmission = 0.0
             N = int(N)
             for i in range(N):
                 if (isotropic):
                     mu = random.random()
                 else:
                     mu = 1.0
                 x = 0
                 alive = 1
                 while (alive):
                     #get distance to collision
                     l = -math.log(1-random.random())*iSig_t
                     #move particle
                     x += l*mu
                     #still in the slab?
                     if (x>thickness):
                         transmission += 1
                         alive = 0
                     elif (x<0):
                         alive = 0
                     else:
                         #scatter or absorb
```

```
                if (random.random() < Sig_s*iSig_t):
                    #scatter, pick new mu
                    mu = random.uniform(-1,1)
                else: #absorbed
                    alive = 0
    transmission /= N
    return transmission
```

As a test, this should do the same thing as the previous example, if we set $\Sigma_s = 0$ and $\Sigma_a = 2$. The scattering ratio in this case is 0 so that all the collisions are absorption, and as result, we just need to track distance to collision.

```
In [10]: N = 100000
         Sigma_s = 0.0
         Sigma_a = 2.0
         transmission = slab_transmission(Sigma_s,Sigma_a, thickness, N,
                                          isotropic=True)
         print("Out of",N,"neutrons only",int(transmission*N),
               "made it through.\n The fraction that made it through was",
               transmission)

Out of 100000 neutrons only 25 made it through.
 The fraction that made it through was 0.00026
```

That seems to be working in that it is close to the answer we saw before. It would be a good idea to run this with larger values of N to show we converge to the correct answer. Forgoing that for now, we will try the problem with $\Sigma_s = 0.75$ and $\Sigma_a = 1.25$. In this case we would expect the transmission rate to go up because the total macroscopic cross-section is the same, but the scattering ratio is greater than zero.

```
In [11]: N = 1000000
         Sigma_s = 0.75
         Sigma_a = 2.0 - Sigma_s
         transmission = slab_transmission(Sigma_s,Sigma_a, thickness,
                                          N, isotropic=True)
         print("Out of",N,"neutrons only",int(transmission*N),
              "made it through.\n The fraction that made it through was",
              transmission)

Out of 1000000 neutrons only 861 made it through.
 The fraction that made it through was 0.000861
```

In this result we see about a factor of three increase. With scattering it takes much longer to do the simulation because we might have to follow each neutron for several steps when we follow it until it is absorbed or leaves the slab. An exercise at the end of the chapter explores this further.

Slab transmission with scattering is a problem where we cannot write down the answer easily. As I mentioned, diffusion cannot solve this problem accurately because it is a boundary driven problem with, potentially, a small amount of scattering. To derive the full solution to the transport equation is beyond the scope of this class, and requires sophisticated mathematics such as singular eigenfunction expansions [23,24]. It is not a stretch to say in this case that the Monte Carlo approach is much easier.

21.7 TRACKING IN A SPHERE

We would like to be able to track in geometries other than slab geometry. One common geometry is a sphere. We will consider a spherical shell around an isotropic source and compute the number of neutrons that escape through the outer radius. We have to be careful because in this geometry a neutron that exits the inner radius will strike the shell on the other side.

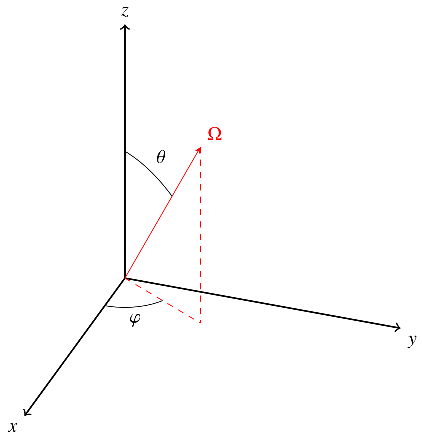
Consider a spherical shell of inner radius, R_i, and outer radius R_o. Neutrons initially strike R_i with a direction given by the vector $\Omega = (\theta, \varphi)$. These directions are defined so that

$$\Omega \cdot \hat{x} = \sin\theta\cos\varphi, \qquad \Omega \cdot \hat{y} = \sin\theta\sin\varphi,$$
$$\Omega \cdot \hat{z} = \cos\theta.$$

The ranges of the angles are $\theta \in [0, \pi]$ and $\varphi \in [0, 2\pi]$ and $\hat{x}, \hat{y}, \hat{z}$ are the unit vectors in the x, y, and z directions. Using these definitions we know that if a neutron travels a distance s, its position changes by

$$\Delta x = s\sin\theta\cos\varphi, \qquad \Delta y = s\sin\theta\sin\varphi,$$
$$\Delta z = s\cos\theta.$$

This coordinate system is shown in the figure below.



One more geometric idiosyncrasy with spherical shells that we have to deal with is the neutrons that cross the inner radius of the shell. They will strike the inner radius again at the other side of the shell. To find where it will strike the inner radius again we need to find the value of s such that

$$(x_i + s\sin\theta\cos\varphi)^2 + (y_i + s\sin\theta\sin\varphi)^2 + (z_i + s\cos\theta)^2 = R_i^2,$$

where (x_i, y_i, z_i) is the point where the neutron is. We could solve this quadratic equation for s, but this is an opportunity to use a root finding method (such as Ridder's method) to find s. I will choose a closed root finding method, like Ridder's method, in this case because the quadratic could have two solutions and I want to make sure that I get an answer between $s = 0$ and $2R_i$. I have saved the `ridder` function that we previously saw in the file `ridder.py`, and I will import that function below.

We now have everything we need for our Monte Carlo program. We will create neutrons initially at R_i. Given the symmetry of the sphere we can set $z = R_i$ and $y = x = 0$ initially. This will mean that the neutrons will have $\theta \in [0, \pi/2]$ initially (otherwise the neutron will not enter the shell). We then sample a distance to collision, s, much like we did before and follow the neutron around. Now at each step we need to update x, y, and z, and check the radius that the neutron is at to make sure it is still in the shell.

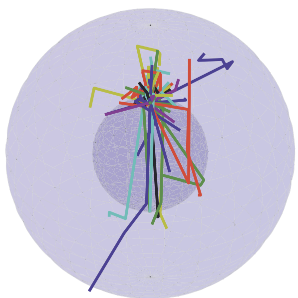
The code to do this is below.

```
In [12]:from ridder import ridder
        def shell_transmission(Sig_s,Sig_a,Ri,Ro,N):
            """Compute the fraction of neutrons that leak through a slab
            Inputs:
            Sig_s:      The scattering macroscopic x-section
            Sig_a:      The absorption macroscopic x-section
            Ri:         Inner radius of the shell
            Ro:         Outer radius of the shell
            N:          Number of neutrons to simulate

            Returns:
            transmission:  The fraction of neutrons that made it through
            """
            Sig_t = Sig_a + Sig_s
            iSig_t = 1/Sig_t
            transmission = 0.0
            N = int(N)

            for i in range(N):
                #get initial direction
                theta = random.uniform(0,0.5*np.pi)
                phi = random.uniform(0,2*np.pi)
                r = Ri
                z = Ri
                x = 0
                y = 0
                alive = 1
                #vector to keep track of positions
                xvec = x*np.ones([1])
                yvec = y*np.ones([1])
                zvec = z*np.ones([1])
                while (alive):
                    #get distance to collision
                    s = -math.log(1.0-random.random())*iSig_t
                    #move particle
                    z += s*math.cos(theta)
                    y += s*math.sin(theta)*math.sin(phi)
                    x += s*math.sin(theta)*math.cos(phi)
                    xvec = np.append(xvec,x)
                    yvec = np.append(yvec,y)
                    zvec = np.append(zvec,z)
```

```
            r = math.sqrt(z**2 + y**2 + x**2)
            #still in the shell?
            if (r>Ro):
                transmission += 1
                alive = 0
            elif (r<Ri):
                #find s so that the neutron is on the other side of the shell
                f = lambda s: ((x + s*math.sin(theta)*math.cos(phi))**2 +
                               (y+s*math.sin(theta)*math.sin(phi))**2 +
                               (z + s*math.cos(theta))**2 - Ri**2)
                s = ridder(f,1e-10,2*Ri,1.0e-10)
                z += s*math.cos(theta)
                y += s*math.sin(theta)*math.sin(phi)
                x += s*math.sin(theta)*math.cos(phi)
                r = Ri

                #check that we are on the inner radius
                assert(math.fabs(x**2+y**2+z**2 - Ri**2) < 1e-6)

            else:
                #scatter or absorb
                if (random.random() < Sig_s*iSig_t):
                    #scatter, pick new angles
                    theta = random.uniform(0,math.pi)
                    phi = random.uniform(0,2*math.pi)
                else: #absorbed
                    alive = 0
    transmission /= N
    return transmission
```

We will simulate transmission through a shell of thickness 3 cm and inner radius 2 cm. Also, we will visualize the tracks that the neutrons take through the shell.

```
In [13]: N = 100
        Sigma_s = 1.0
        Sigma_a = 1.0
        Ri = 2
        Ro = Ri + 3
        transmission = shell_transmission(Sigma_s,Sigma_a,Ri,Ro,N)
        print("Out of",N,"neutrons only",int(transmission*N),
              "made it through.\n The fraction that made it through was",
              transmission)
```



```
Out of 100 neutrons only 1 made it through.
 The fraction that made it through was 0.01
```

Notice that all the neutrons start at $z = R_i$ and $x = y = 0$ as prescribed in the code. We can also see the fact that when a neutron re-enters the hollow center, it streams across to the other side. This figure is also a way to check that the streaming through the hollow part of the shell is handled correctly: we should not see any neutron tracks end in the hollow part of the sphere (though this is hard to tell with a 2-D projection of the sphere). We can also see the one neutron that escaped the sphere.

Upon increasing the number of neutrons, we expect to get a more accurate answer, though we have not said what that answer is. With $N = 10^5$ we get

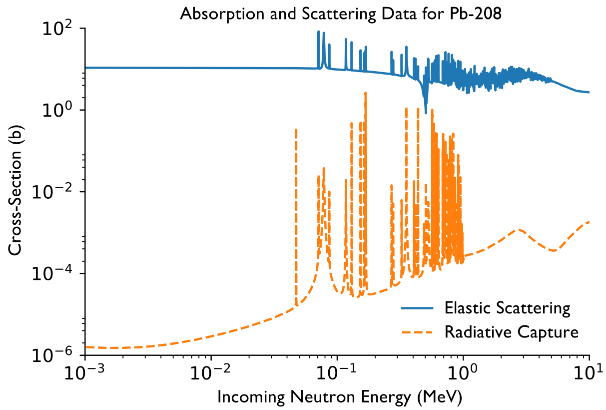
```
In [14]: N = 10**5
        transmission = shell_transmission(Sigma_s,Sigma_a,Ri,Ro,N)
        print("Out of",N,"neutrons only",int(transmission*N),
              "made it through.\n The fraction that made it through was",
              transmission)

Out of 100000 neutrons only 602 made it through.
 The fraction that made it through was 0.00602
```

21.8 A REAL SHIELDING PROBLEM

We will now take a large step forward. We will try to solve the problem of designing a lead-208 shield for a bare reactor made of uranium-235. We will use the full energy dependent cross-sections for lead and the actual fission spectrum of U-235. To do this we will have to read in the data for the lead microscopic cross-sections and the fission spectrum. We covered how to do this in Section 5.1. Using that knowledge we can read in a csv file of the format: incident neutron energy, cross-section in barns (10^{-24} cm^2). The code below does this. A plot of the cross-sections follows.

```
In [15]: import csv
         lead_s = [] #create a blank list for the x-sects
         lead_s_energy = [] #create a blank list for the x-sects energies
         #this loop will only execute if the file opens
         with open('pb_scat.csv') as csvfile:
             pbScat = csv.reader(csvfile)
             for row in pbScat: #have for loop that loops over each line
                 lead_s.append(float(row[1]))
                 lead_s_energy.append(float(row[0]))
         lead_scattering = np.array([lead_s_energy,lead_s])
         lead_abs = [] #create a blank list for the x-sects
         lead_abs_energy = [] #create a blank list for the x-sects energies
         #this loop will only execute if the file opens
         with open('pb_radcap.csv') as csvfile:
             pbAbs = csv.reader(csvfile)
```

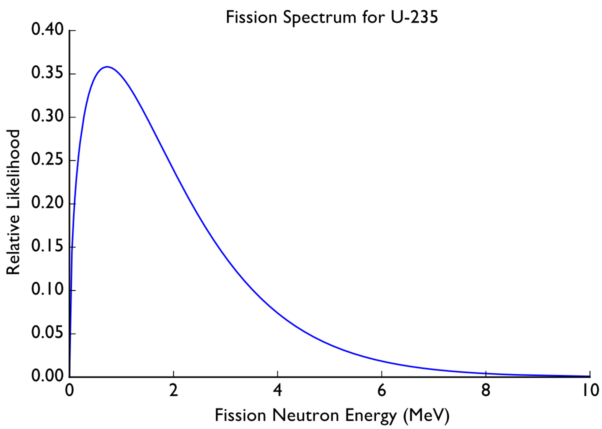
```
    for row in pbAbs: #have for loop that loops over each line
        lead_abs.append(float(row[1]))
        lead_abs_energy.append(float(row[0]))
lead_absorption = np.array([lead_abs_energy,lead_abs])
```



For the fission spectrum we will use the Watt fission spectrum. This spectrum is the relative likelihood of a fission neutron being born with energy E. The fission spectrum is typically denoted as $\chi(E)$ and given by

$$\chi(E) = 0.453e^{-1.036E}\sinh\left(\sqrt{2.29E}\right),$$

with E given in MeV.

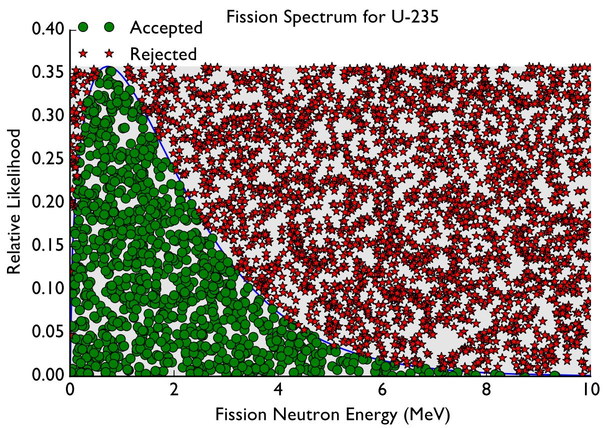


To solve this problem we will have to change our algorithm somewhat. Firstly, we will have to generate neutrons with energies sampled from the fission spectrum and then evaluate the cross-sections at the neutron's energy. Secondly, we will have to change how we scatter particles. When a particle scatters we will have to sample a new energy for the post-scattered neutron. We will tackle each of these next.

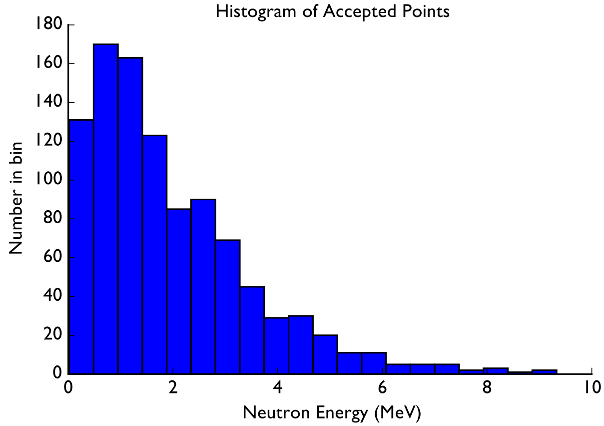
21.9 REJECTION SAMPLING

Previously, we discussed how to sample from a distribution by inverting the CDF and then using a random number between 0 and 1 to give us the inverse CDF value corresponding to our sample. With the fission spectrum we cannot do this easily. We do not have a CDF, we just have a distribution that gives a relative likelihood of a fission neutron being born with a certain energy. To sample from this we use rejection sampling. The idea of rejection sampling is to draw a box around the PDF of the distribution we want to sample from, and pick points in the box. If the point is below the curve, we accept the point, otherwise we reject it and sample again. The effect of this is that we will get more points where the PDF is large, and few points where the PDF is small.

We will demonstrate the idea of rejection sampling with our fission spectrum data. To do this we find the maximum and the minimum of the function over the energy range from the minimum energy in the lead scattering table to 10 MeV. This allows us to define the box, and we randomly pick points in the box. Then we check to see if a point is above or below the function.



The histogram of the accepted samples should look like the fission spectrum we wanted to sample. The histogram will not be perfect because we have a finite number of samples.



BOX 21.3 NUMERICAL PRINCIPLE

To generate samples from a distribution where you cannot invert the CDF, $F(x)$, you can use rejection sampling. To generate a sample, first pick a value $\hat{x}$ randomly between the minimum possible and maximum possible value of x. Then pick a value $\hat{y}$ randomly between 0 and the maximum value of the PDF. If $\hat{y} < f(\hat{x})$, where $f(x)$ is the PDF, then $\hat{x}$ is accepted as a sample. Otherwise, $\hat{x}$ is rejected, and we try again.

21.10 LOOKING UP ENERGIES

To look up the cross-section for lead at different energies we need a function that can return the value of the cross-section for a given energy. We can make this happen by finding the energy in the data set that is closest to the input energy. This can be done using the NumPy function `argmin`. This function returns the index of a NumPy array with the smallest value. Therefore, we pass to `argmin` the difference between a target energy and the vector of energies in the table. In effect for a given neutron energy this will give the point in the table closest to that energy. We define such an energy lookup function below.

```
In [16]: def energy_lookup(data_set, inp_energy):
             """look up energy in a data set and
             return the nearest energy in the table
             Input:
             data_set:   a vector of energies
             inp_energy: the energy to lookup

             Output:
             index: the index of the nearest neighbor in the table
             """
             #argmin returns the indices of the smallest members of an array
```

```
    #here we'll look for the minimum difference
    #between the input energy and the table
    index = np.argmin(np.fabs(data_set-inp_energy))
    return index
```

21.11 ELASTIC SCATTERING

When a particle scatters elastically, the energy of the scattered neutron, E', of a neutron with an initial energy E is governed by a probability given by

$$P(E \to E') = \begin{cases} \frac{1}{E(1-\alpha)} & \alpha E \le E' \le E \\ 0 & \text{otherwise} \end{cases},$$

where

$$\alpha = \frac{(A-1)^2}{(A+1)^2},$$

with A the mass of the nucleus. Therefore, we can sample the value of the scattered neutron's energy from a uniform distribution from αE to E. The neutron's angle would also be a function of the scattered energy, in order to preserve momentum. For simplicity we will say that the neutron's angle after the scatter is isotropic, though this is not completely correct. The proper scattering would give a particular value of μ for a given energy change.

21.12 LEAD SHIELDING OF REACTOR ALGORITHM AND CODE

The algorithm will be an enhanced version of the one before that concerned neutrons striking an absorbing and scattering slab. We will assume isotropic, elastic scattering and radiative capture as the only reactions in the lead, though this simplification could be modified using the additional cross-sections for inelastic scattering, $(n, 2n)$ reactions, etc. The algorithm now looks like:

1. Create a neutron with μ sampled from the uniform distribution $\mu \in [0, 1]$ and an energy sampled from the fission spectrum via rejection sampling. Set $x = 0$.
2. Sample randomly a distance to collision, l, from the exponential distribution.
3. Move the particle to $x = x + l\mu$.
4. Check to see if x is greater than the shield thickness, if so stop following the neutron. Check if $x < 0$, if so go to 1.
5. Sample a random number s in [0,1], if $s < \Sigma_s/\Sigma_t$, the particle scatters and sample $\mu \in [-1, 1]$ and an energy in based on the formula above and go to step 3. Otherwise, continue.
6. Go back to 1 until we have run "enough" neutrons.

The resulting function is given below.

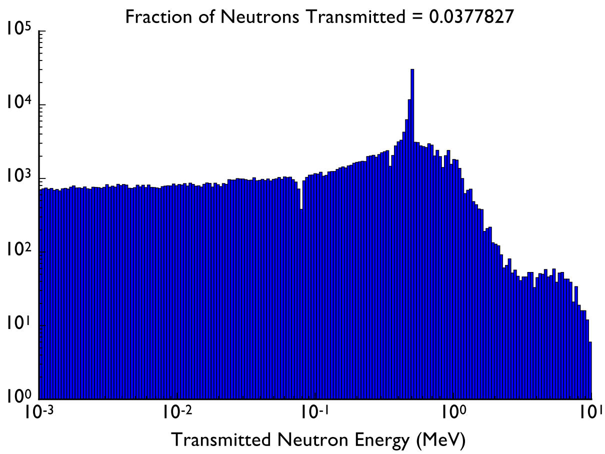
```
In [17]: def slab_reactor(sig_s,sig_a,thickness,density,A,N,isotropic=False):
             """Compute the fraction of neutrons that leak through a slab
             Inputs:
             sig_s:     The scattering microscopic x-section array in form Energy,
                        X-sect
             sig_a:     The absorption microscopic x-section
             thickness: Width of the slab
             density:  density of material in atoms per cc
             A:         atomic weight of shield
             N:         Number of neutrons to simulate
             isotropic: Are the neutrons isotropic or a beam

             Returns:
             transmission:  energies of neutrons that leak through
             created:  energies of neutrons that were born
             """
             alpha = (A-1.0)**2/(A+1.0)**2
             Sig_s = sig_s.copy()
             Sig_a = sig_a.copy()
             Sig_s[1,:] = density/1e24*Sig_s[1,:]
             Sig_a[1,:] = density/1e24*Sig_a[1,:]
             #make rejection box
             min_eng = np.min([np.min(Sig_s[0,:]),np.min(Sig_a[0,:])])
             max_eng = np.max([np.max(Sig_s[0,:]),np.max(Sig_a[0,:])])
             max_prob = np.max(np.max(expfiss(Sig_a[0,:])))
             transmission = []
             created = []
             N = int(N)
             for i in range(N):
                 #sample direction
                 if (isotropic):
                     mu = random.random()
                 else:
                     mu = 1.0
                 #compute energy via rejection sampling
                 rejected = 1
                 while (rejected):
                     #pick x
                     x = random.uniform(min_eng,max_eng)
                     y = random.uniform(0,max_prob)
                     rel_prob = expfiss(x)
                     if (y <= rel_prob):
                         energy = x
                         rejected = 0
                 #initial position is 0
                 x = 0
                 created.append(energy)
                 alive = 1
                 while (alive):
                     #get distance to collision
                     scat_index = energy_lookup(Sig_s[0,:],energy)
                     abs_index = energy_lookup(Sig_a[0,:],energy)
                     cur_scat = Sig_s[1,scat_index]
                     cur_abs = Sig_a[1,abs_index]
```

```
                Sig_t = cur_scat + cur_abs
                l = -math.log(1-random.random())/Sig_t
                #move particle
                x += l*mu
                #still in the slab
                if (x>thickness):
                    transmission.append(energy)
                    alive = 0
                elif (x<0):
                    alive = 0
                else:
                    #scatter or absorb
                    if (random.random() < cur_scat/Sig_t):
                        #scatter, pick new mu and energy
                        mu = random.uniform(-1,1)
                        energy = random.uniform(alpha*energy,energy)
                    else: #absorbed
                        alive = 0
        return transmission, created
```

This algorithm will be more time consuming to run because tracking each neutron now requires more work (e.g., we have to perform rejection sampling to get an initial energy), and the fact that the scattering ratio for lead appears to be high from the figure above. We will run the algorithm with only one million neutrons. Before running the code, we need to compute the number density for lead-208 because the algorithm takes the microscopic cross-section as an input and multiplies that by a number density to get the macroscopic cross-section.

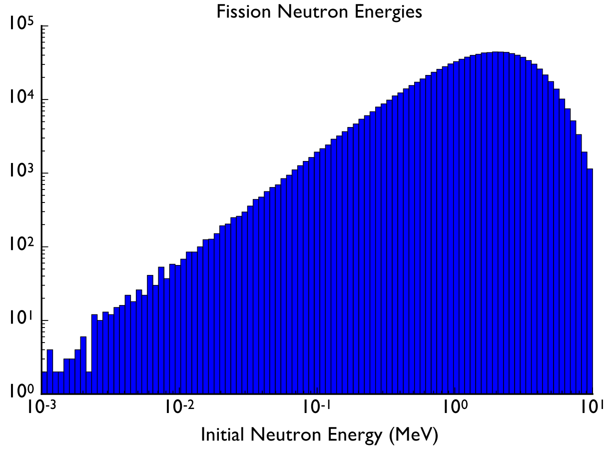
```
In [18]: N = 1e7
         density = 11.34/208*6.022e23
         thickness = 150
         transmission,created = slab_reactor(lead_scattering,lead_absorption,
                                             thickness,density,208, N,
                                             isotropic=True)
```

The output of the function is an array of the transmitted particle energies and the initial energies. The distribution of the transmitted energies is



The result is that about 3.77% of the incident neutrons transmit through the shield (making this not a very good shield). There are some interesting phenomenon that we can observe in the transmitted neutrons. In particular, the peaks and valleys of the radiative capture cross-section are mimicked in the transmitted neutron energies.

The neutrons that entered the slab, as function of energy as sampled from the fission spectrum, are shown in the next histogram. With a logarithmic scale, the fission spectrum will look a bit different.



As we would expect, the transmitted energies are a blend of the incident energies and the cross-sections. We could modify this problem by adding other materials, making the shield thicker, or other modifications to improve the shield if we desired. The basics of the algorithm will not change.

CODA

We have demonstrated that we can solve complicated problems by “rolling dice” if we roll many, many dice and move particles around based on these random numbers. One feature of this approach is that it requires little in the way of mathematical sophistication, with the tradeoff that the convergence is slow (remember that the noise in the solution decays as the number of samples to the negative one-half power). Nevertheless, Monte Carlo methods are attractive and they are widely used in nuclear engineering and other fields. In the next two chapters we will expand our Monte Carlo capabilities. In the next chapter we will go over how to reduce the run-to-run variability of Monte Carlo calculations, and provide ways to estimate the scalar flux of neutrons in a system.

FURTHER READING

The Monte Carlo method is a rich subject in nuclear engineering. For a more detailed coverage of the topic we encourage the reader to read one of the monographs devoted to the topic. Two good examples are the recent book by Dunn and Shultis [25] or the work of Kalos and Whitlock [26].

PROBLEMS

Short Exercises

21.1. Consider a beam of neutrons striking a slab of thickness 5 cm and $\Sigma_t = 1.0\ \text{cm}^{-1}$. Compute the transmission fraction and time how long the calculation takes using $N = 10^6$ neutrons and several different scattering ratios: 0, 0.1, 0.5, 0.9, 1.0. Compare your computed transmission fractions as a function of scattering ratio to the expected trend as the scattering is increased.

21.2. Modify the shielding code to consider neutrons of a single energy impinging on the shield and to tally the energy of the absorbed neutrons. Assume the neutrons are all 2.5 MeV and are produced from the fusion of deuterium. Plot the distribution of transmitted and absorbed neutrons with a large enough number of sampled neutrons.

21.3. The Maxwell–Boltzman distribution, often called just a Maxwellian distribution, gives the distribution of speeds of particles in a gas by the formula

$$f(v) = \sqrt{\left(\frac{m}{2\pi kT}\right)^3} 4\pi v^2 e^{-\frac{mv^2}{2kT}}$$

where m is the mass of the particles, T is the temperature, and k is the Boltzmann constant. Consider a gas of deuterium at $kT = 1\ \text{keV} = 1.60218 \times 10^{-16}$ J. Sample particle speeds from the Maxwellian using rejection sampling. From your sampled points, compute the mean speed and the square-root of the mean speed squared (i.e., compute the mean value of the speed squared and then take the square root, aka the root-mean square speed). The mean speed should be

$$\int_0^\infty dv\, v f(v) = \sqrt{\frac{8kT}{\pi m}},$$

and the root-mean square speed should be

$$\sqrt{\int_0^\infty dv\, v^2 f(v)} = \sqrt{\frac{3kT}{m}}.$$

Compute these quantities using sample numbers of $N = 10, 10^2, 10^3, 10^4, 10^5$ and discuss your results.

Programming Projects

1. Monte Carlo Convergence

In this exercise you will demonstrate the standard deviation of the estimates decays as $N^{-1/2}$. Solve the problem of a beam striking an absorbing slab, $\Sigma_\mathrm{t} = \Sigma_\mathrm{a} = 1.0\ \mathrm{cm}^{-1}$, with thickness 3 cm. Solve this problem with $N = 10^2, 10^3, 10^4, 10^5, 10^6$. At each value of N estimate the solution 10 times, and take the standard deviation of the estimates. Plot the standard deviation as a function of N on a log-log scale. Compare your results to the expected trend.

2. Track-Length in Sphere

Consider a solid sphere of radius R that has neutrons born isotropically in angle and uniformly in space inside of the sphere. Assuming that no neutrons collide in the sphere, using Monte Carlo compute the average distance the neutron travels inside of the sphere before exiting the sphere. Compute this for several values of R and see if you can find a trend.