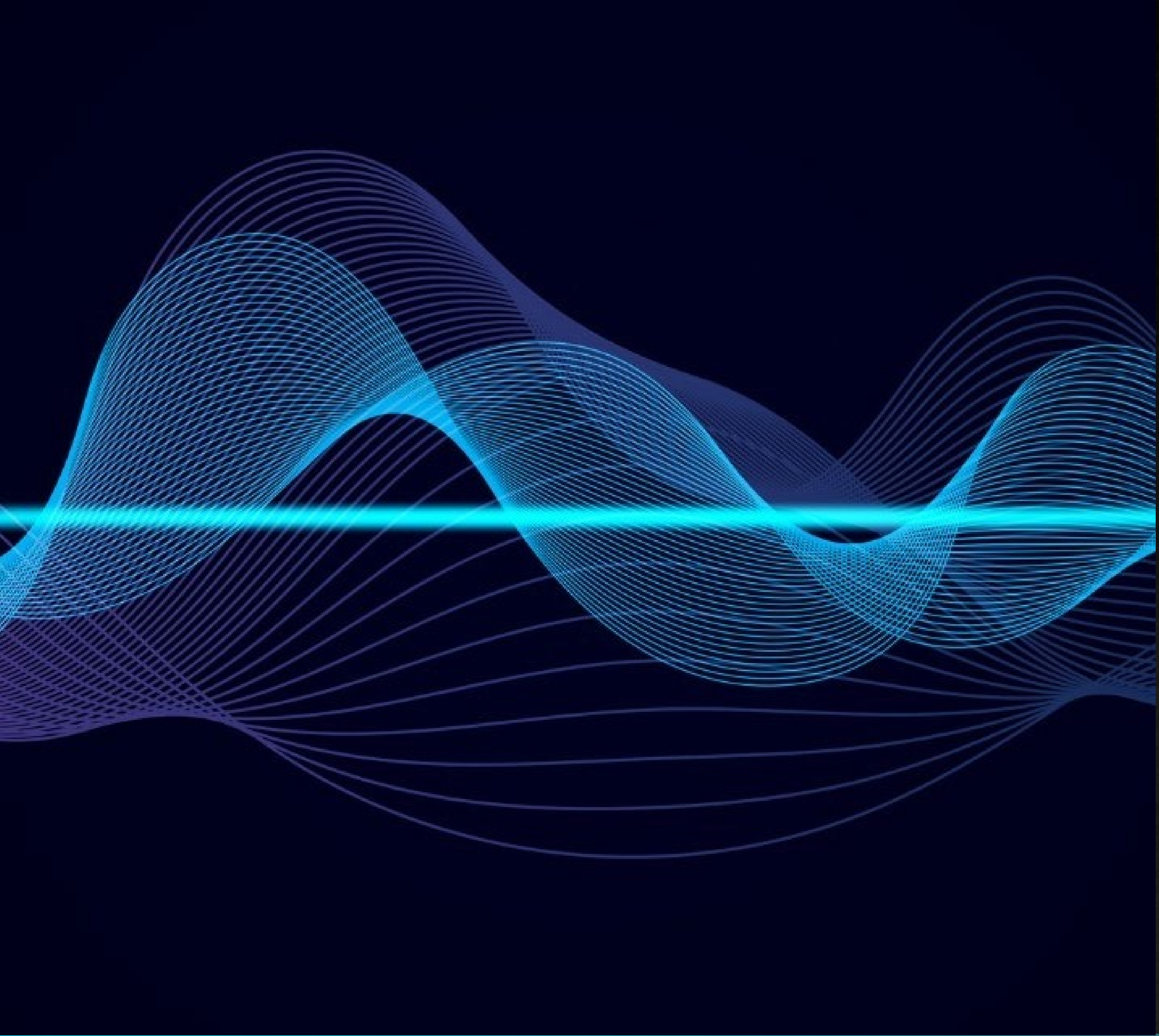


Computational Physics

PHYS 6260

Random Processes

Announcements:

- HW3: Due Friday 1/31

Lecture Outline

We will cover these topics

- Random number generators
- Non-uniform random numbers
- Gaussian random numbers

Introduction

- There are some random processes in physics.
- For example, quantum processes in radioactive decay and electrons transitioning into the ground state
- If we know the probability per unit time, we can use that info in the calculation

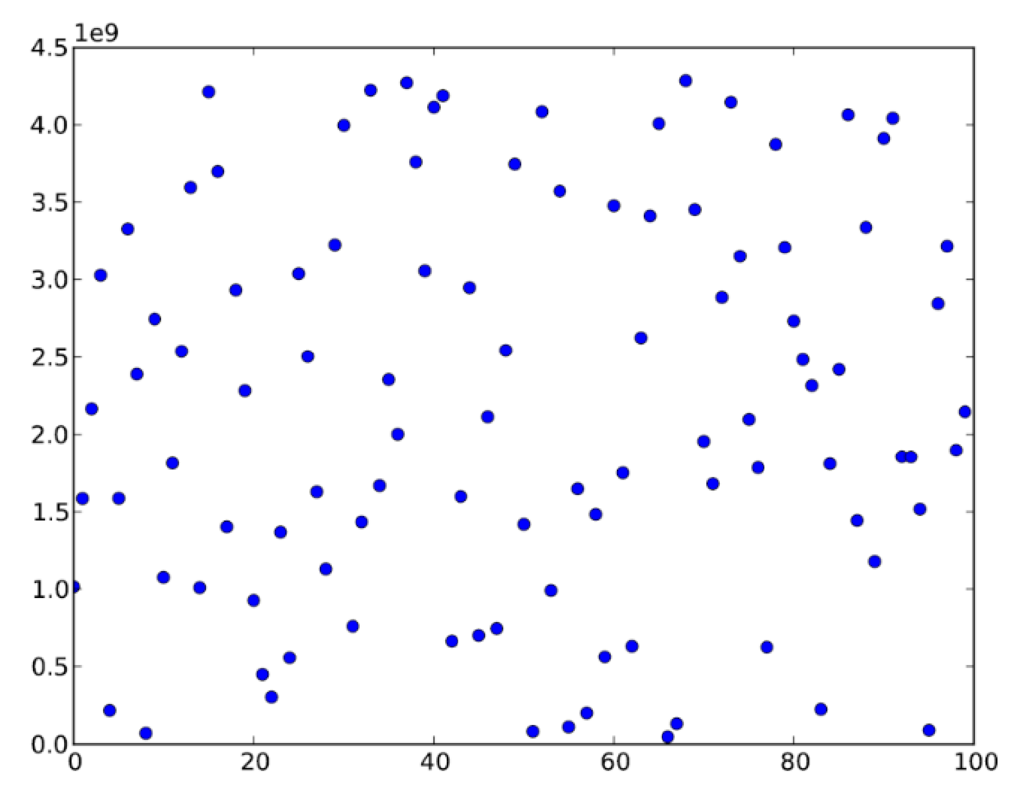
- There are non-uniform processes that can modeled as random
- For example, Brownian motion of a particle seems like a random process, but it depends on the initial positions and velocities of the particles
- Modeling all particles would be computationally intractable, but we can model it as a random process and it works surprisingly well

Random numbers

- The most basic random number generator (RNG) starts with an integer (known as a seed) and generates numbers from it
- For example, $x' = (ax + c) \bmod m$ takes some number x and generates a new number x'. (a,c,m) are integer constants
- The random sequence depends on the seed
  - It is reproducible
  - Known as a linear congruent RNG

Random numbers

- The figure shows the random numbers generated from this example
- Notice that
  - The sequence is not random but deterministic, depending on the seed
  - The values will be within [0, m-1]
  - The values of a, c, m are carefully chosen
    - Otherwise, the number distribution could have biases
    - Here, c is prime, a only has three factors, and $m = 2^{32}$



- In general, linear congruential generators produce pretty bad random numbers because there are correlations between the numbers

Random numbers

- For high-quality calculations, the RNG should have little to no correlation between numbers
- The most widely-used RNG is known as the Mersenne twister
  - Computationally cheap and easy to implement
  - Default RNG in `numpy.random.random()`
  - See this page for all of the available routines

- Numpy's random() will give a uniformly distributed random number between 0.0 and 1.0
- Takes an optional argument of the size of returned array
  - For example, an argument of (3,10) will give a 3x10 random array of floats between 0 and 1
- If no argument is given, the output is scalar

Example: Probabilities & biased coins

- In various physics calculations, events can have some probability p to occur
- For example, a particle could have a 20% chance to move or remain stationary otherwise
- This is known as the "toss of a biased coin"
- It is very straightforward to implement

```python
from numpy.random import random
if random() < 0.2:
    print("Heads")
else:
    print("Tails")
```

Decay of an isotope

In-class problem

- Radioactive isotopes have some probability per unit time to decay into another isotope
- ^{210}Tl (thallium) decays into stable ^{208}Pb (lead) with a half-life $\tau = 183.2$ s
- On average, the number N of original atoms will exponentially decrease as $N(t) = N(0)2^{-t/\tau}$
- Within some time interval t, the probability that a single atom has decayed is $p(t) = 1 - 2^{-t/\tau}$

- We can simulate this random process by dividing N = 1000 atoms into two sets: thallium and lead
- Initially it's all thallium. Advance the system with a timestep of 1 s, in which we decide how many atoms decay into lead
- Perform the calculation for 1000 seconds and plot the populations as a function of time

Non-uniform random numbers

- Most random processes in physics have some non-uniformity to them
- Like some dependence on energy, position, or velocity
- Let’s go back to our radioactivity decay example

- A single atom has a probability to decay in a time interval t of $1 - 2^{-t/\tau}$
- For some small time interval dt, this probability is

$$1 - \exp\left(-\frac{dt}{\tau}\ln 2\right) = \frac{\ln 2}{\tau}\,dt$$

- Here we took the Taylor expansion of exp and neglected terms dt^2 and higher terms

Non-uniform random numbers

$$1 - \exp\left(-\frac{dt}{\tau}\ln 2\right) = \frac{\ln 2}{\tau}\,dt$$

- **What's the decay probability between times t and t+dt?**
- For an atom to decay within that interval, it must survive until time t
  - This probability is $2^{-t/\tau}$
- Thus the total probability P(t)dt of decay during this interval is

$$P(t)dt = 2^{-t/\tau}\frac{\ln 2}{\tau}\,dt$$

- This is a clear example of a non-uniform probability distribution
- Here atoms have a higher probability of decaying earlier than later

- Now we don't have to step forward in time
- We simply draw random numbers from the P(t) distribution. But how?

Non-uniform random numbers

- Generate a set of uniform random numbers z with some probability density q(z)
- Transform them into a non-uniform set p(x), using a function x(z)
- Goal: Choose x(z) so that x has the distribution p(x) we desire

- Probability of generating a number between x and x+dx is equal to generating a value z within a corresponding interval: p(x)dx = q(z)dz
- For a numpy's random(), q(z) = 1 between 0 and 1, and zero otherwise
- Integrating both sides to some value x(z),

$$\int_{-\infty}^{x(z)} p(x')dx' = \int_0^z dz' = z$$

- Solve for x(z). Not always possible, though

Example: Non-uniform random numbers

$$\int_{-\infty}^{x(z)} p(x')dx' = \int_0^z dz' = z$$

- Suppose that we have the following normalized probability distribution

$$p(x) = \mu e^{-\mu x}$$

- Using the equation above, we find

$$\mu \int_0^{x(z)} e^{-\mu x'}\, dx' = 1 - e^{-\mu x} = z$$

- Solving for x

$$x = -\frac{1}{\mu}\ln(1 - z)$$

- Given this, we draw numbers from a uniform distribution and plug them into this equation

Gaussian random numbers

$$\int_{-\infty}^{x(z)} p(x')dx' = \int_0^z dz' = z$$

- In many fields of physics, processes often generate Gaussian probabilities (e.g. Maxwellian velocity distributions)

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right)$$

- Applying this function to our non-uniform treatment, we arrive at

$$\frac{1}{\sqrt{2\pi\sigma^2}} \int_0^x \exp\left(-\frac{x^2}{2\sigma^2}\right) dx = z$$

- This cannot be solved analytically, but there is a workaround

Gaussian random numbers

$$\frac{1}{\sqrt{2\pi\sigma^2}}\int_0^x \exp\left(-\frac{x^2}{2\sigma^2}\right) dx = z$$

- Imagine we have two independent random numbers, [x,y], both drawn from the same Gaussian distribution
- The probability that this point falls within an element dxdy at point (x,y) is

$$p(x)p(y)dxdy = \frac{1}{2\pi\sigma^2}\exp\left(-\frac{x^2+y^2}{2\sigma^2}\right) dx\, dy$$

- This has circular symmetry, and we can re-express it in polar coordinates

$$p(r,\theta)drd\theta = p(r)dr\, p(\theta)d\theta = \frac{r}{\sigma^2}\exp\left(-\frac{r^2}{2\sigma^2}\right) dr \times \frac{d\theta}{2\pi}$$

- Notice that would could separate the variables
- The angle is just a uniformly distributed random number

Gaussian random numbers

$$\frac{1}{\sqrt{2\pi\sigma^2}}\int_0^x \exp\left(-\frac{x^2}{2\sigma^2}\right)dx = z$$

- For the radial component, we have

$$p(r)dr = \frac{r}{\sigma^2}\exp\left(-\frac{r^2}{2\sigma^2}\right)dr$$

- Inserting into the non-uniform transformation, we obtain

$$\frac{1}{\sigma^2}\int_0^r \exp\left(-\frac{r^2}{2\sigma^2}\right)rdr = 1 - \exp\left(-\frac{r^2}{\sigma^2}\right) = z$$

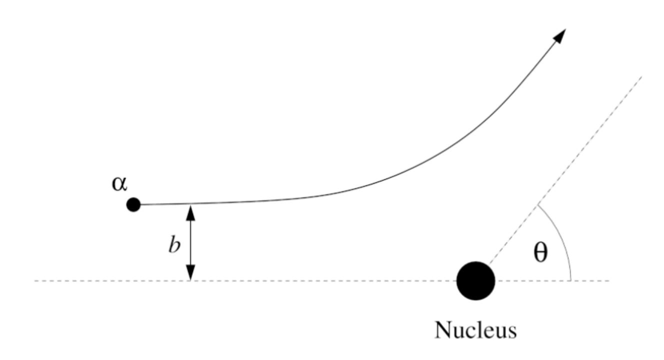
- Solving for r,

$$r = \sqrt{-2\sigma^2 \ln(1-z)}$$

- Here z is a uniformly distributed random number
- Now we have (r, θ) as random numbers and we just convert back to Cartesian

Rutherford Scattering

In-class problem



- This process occurs when positively charged particles (e.g. α-particles) is deflected by an atom by the Coulomb force
- The scattering angle obeys

$$\tan\frac{\theta}{2} = \frac{Ze^2}{2\pi\epsilon_0 E b}$$

- Z is the atomic number, e is the electron charge, E is the kinetic energy, and b is the impact parameter
- Consider a beam of α-particles with a Gaussian profile with a spread $\sigma = a_0/100$, where a_0 is the Bohr radius
- The beam is fired at a gold atom
- Goal: to calculate the fraction of α-particles that back-scatter $\left(\theta > \frac{\pi}{2}\right)$

Recall: $r = \sqrt{-2\sigma^2 \ln(1-z)}$