PHY1610H - Scientific Computing: Randomness

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Today's class

Today we will discuss:

- Randomness, why you want it.
- How to make it or fake it.
- Applications: Monte Carlo

Why Randomness?

Why Randomness?

- To simulate some physical phenomenon that has noise.

  E.g. Brownian motion, Nyquist noise.

  On the level of their description, this is real randomness.

- To perform averages or integrals in systems with many degrees of freedom.

  E.g. Stat. Phys. computations, path integral calculations.

  Here, the main objective is to get the converged answer quickly.

- To estimate a parameter's distribution from using data (MCMC).

- To test a statistical method.

Creating Randomness

Sources of randomness

True Random Number Generators

- Lava lamps.
- Radioactive decay.
- Various quantum processes.
- Atmospheric noise.
- Random computer hardware noise signals (thermals noise).

Generally slow, expensive, impossible to reproduce for debugging. Hard to characterize underlying distribution.

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Pseudo Random Number Generators

- Come up with a algorithm that produces random numbers
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Pseudo Random Number Generators

- Come up with a algorithm that produces random numbers
- But wouldn't such an algorithm would be deterministic?
- Only has to **act** random, i.e., give fair and uncorrelated sequence.

Pseudo Random Number Generators (PRNG)

Recipe:

- Define some ‘state’, initialized by some ‘seed’ value(s).
- Produce a number from this state.
- Advance the state determistically.

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Depends a lot on the way the states are advanced. **Must test.**

Distributions are transformations

- Suppose we had a way to draw random values of a continuous variable x that is uniformly distributed between 0 and 1.
- Let's say that for any value x that is drawn, we were to compute a value $y = f(x)$, where f is a deterministic function.
- The values of y are also randomly distributed, but with a non-uniform distribution (unless $f(x) = x$).

So we can turn a uniformly distributed random variable into a non-uniformly distributed variable by applying a function.

If we want a specific non-uniform distribution, we just need to figure out the function. For many common cases, this is already done.

So our main focus is first to find uniformly distributed variables.

All pseudo random numbers are discrete

Despite the illusion of continous variables that floating point numbers give, there are only a finite number of bits, and thus a discrete set of values.

In fact, routines that give pseudo random floating point numbers are usually based on drawing a random integer number and dividing it by the largest possible generated integer.

From a random integer of n bits, we just need each bit to be uniformly distributed, with a chance of 50% of a 0 and 50% of a 1.

Warning: most PRNGs give lower bits that are more correlated than the higher bits.

Example: Coin Toss

The following class can produce a 'random' 1's and 0's representing heads and tails:

```
// badcoin.h
class BadCoin {
 public:
  // method to set the starting seed
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   state = seed;
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```
#include <iostream>
#include "badcoin.h"
int main()
{
  BadCoin coin;
  coin.start(13); //seed
  // toss the coin 20 times
  for (int i = 0; i < 20; i++)
    std::cout << coin.toss() << '\n';
  return 0;
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- Independent samples?

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1. Fairness: histogram counting the occurance of values

$$h_x = \sum_{i=1}^{N} \delta_{x x_i}$$

Here x is one of the possible random numbers (here ± 1), and x_i are samples produced by our PRNG ($\delta_{ii} = 1, \delta_{i,j\neq i} = 0$).

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2. Independence:

   One way is to look at correlations between samples:
$$c_j = \langle x_i x_{i+j} \rangle = \frac{1}{N} \sum_{i=1}^{N} (x_i - \bar{x})(x_{i+j} - \bar{x})$$
   If independent: $\mathcal{O}(1/\sqrt{N})$ if $j > 0$

Test results (N=20)

Fairness

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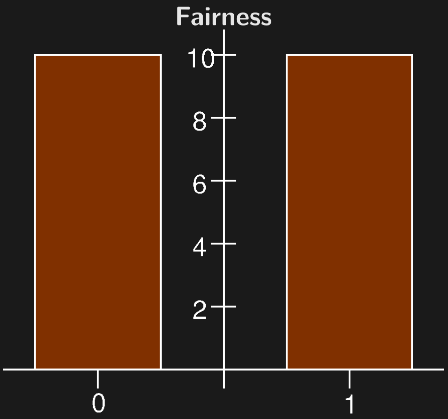

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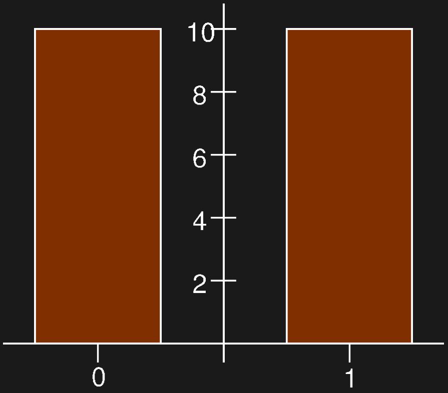

Good!

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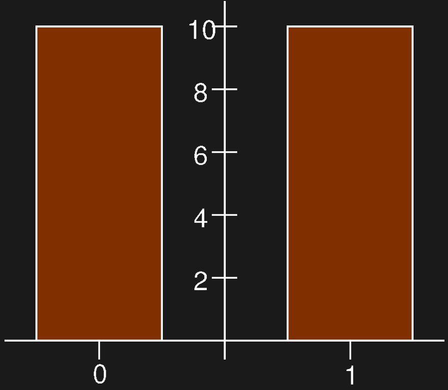

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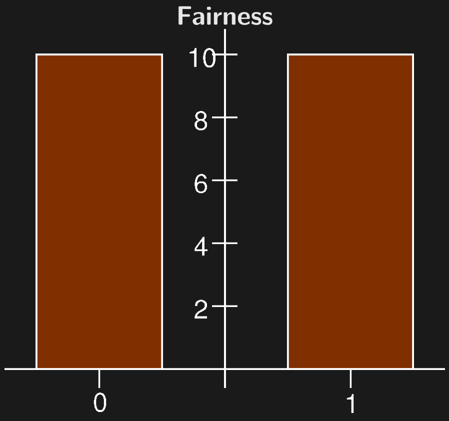

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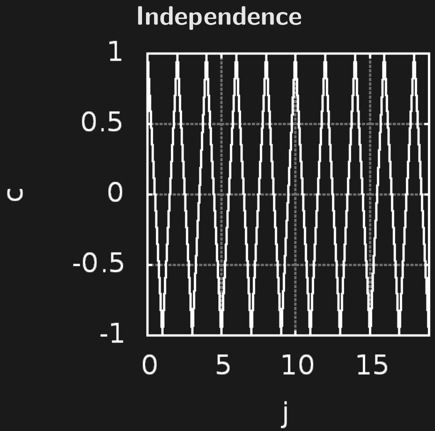

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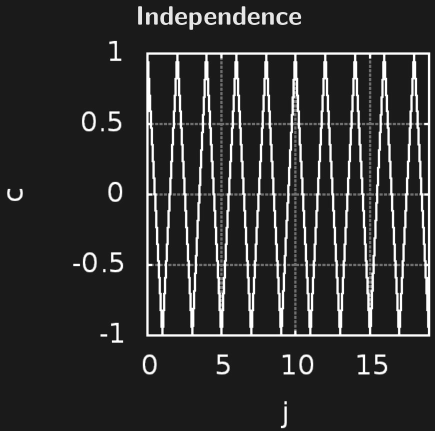
Good!



Bad!

Try again

Old version

```
// badcoin.h
class BadCoin {
 public:
  // method to set the starting seed
  void start(int seed) {
   state = seed;
  }
  // method to toss the coin (1: head, 0: tail)
  int toss() {
   state++; // update state
   return state%2; // using lowest bit...
  }
 private:
  unsigned int state; // internal state
};
```

New version

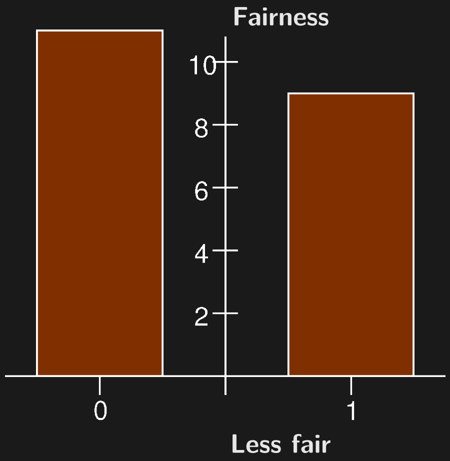
```
// improvedcoin.h
class ImprovedCoin {
 public:
  // method to set the starting seed
  void start(int seed) {
   state = seed;
  }
  // method to toss the coin (1: head, 0: tail)
  int toss() {
   state = 100+100*sin(state+1); // update state
   return state%2; // using lowest bit...
  }
 private:
  unsigned int state;
};
```

Difference lies in the update of the state. Instead of just increasing state, we created a more complicated form, hoping that the complexity will make it more random.

Test results (N=20)

Fairness

Test results (N=20)



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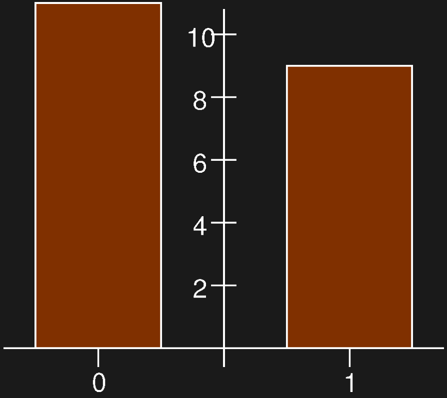

Less fair

Independence

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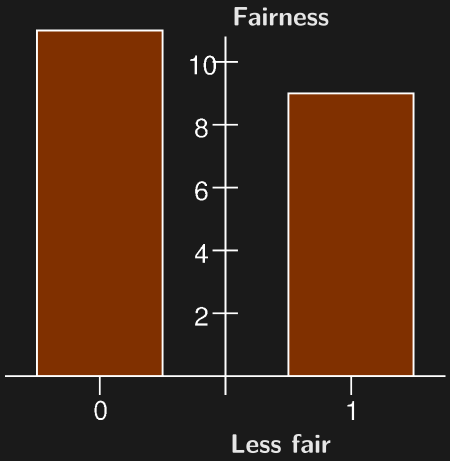

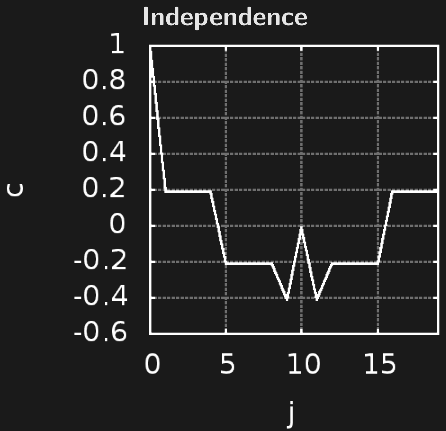

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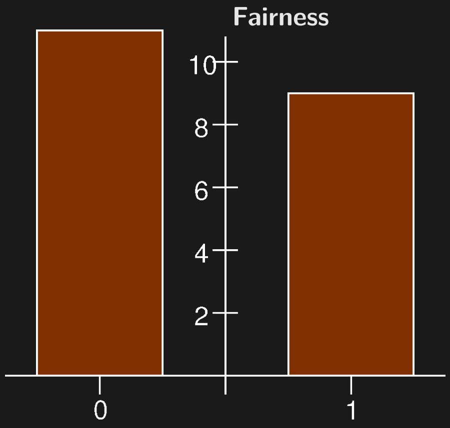
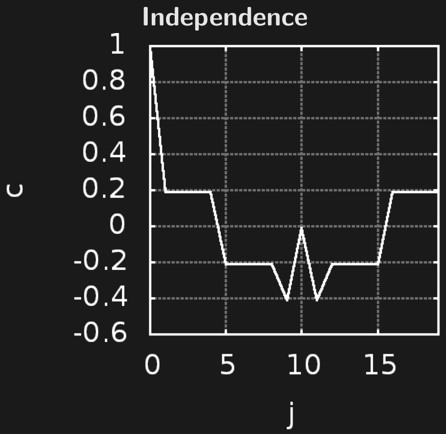


Less fair



Better?

Let's do more samples: N=200

Fairness

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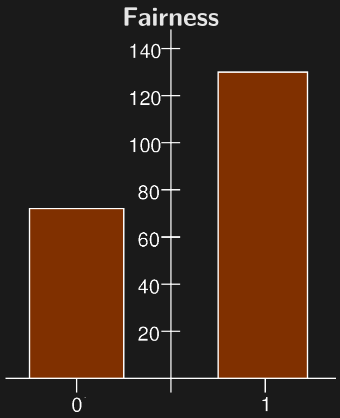
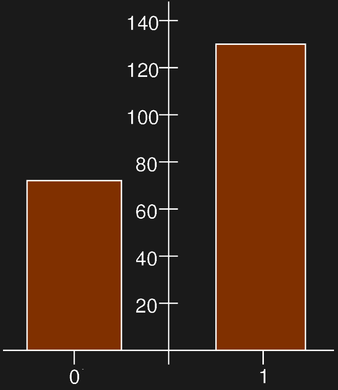


Bad

Let's do more samples: N=200

Fairness



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Independence

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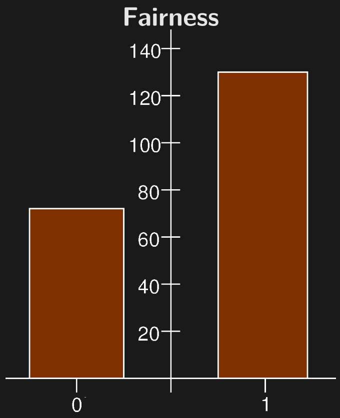

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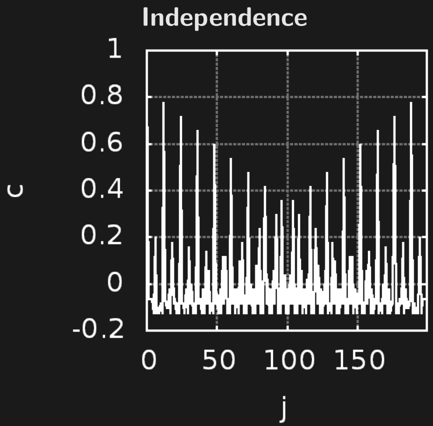

Bad

Moral: Don't do it yourself

What properties do we expect from a random number generator?

- We would like them from a given distribution (uniform, Gaussian).
- We would like them to be unpredictable.
- We would like them to be reproducible.
- We need them to be generated quickly.
- We need to have a long period.

We saw that it is not that easy to guess good PRNG algorithms and parameters

There was a time when one was forced to implement PRNGs oneself, as standard ones were quite bad, but C++11 standard has random number generators in it.

Using existing random numbers

C++11 way

```
// goodcoin.h
#include <random>
class GoodCoin {
 public:
   GoodCoin(): uniform(0,1) {}
   // method to set the starting seed
   void start(int seed) {
     engine.seed(seed);
   }
   // method to toss the coin (1: head, 0: tail)
   int toss() {
     return uniform(engine); // state in engine
   }
 private:
  std::uniform_int_distribution<int> uniform;
  std::mt19937 engine; // PNRG state
};
```

Previous way

```
// improvedcoin.h
class ImprovedCoin {
 public:
  // method to set the starting seed
  void start(int seed) {
   state = seed;
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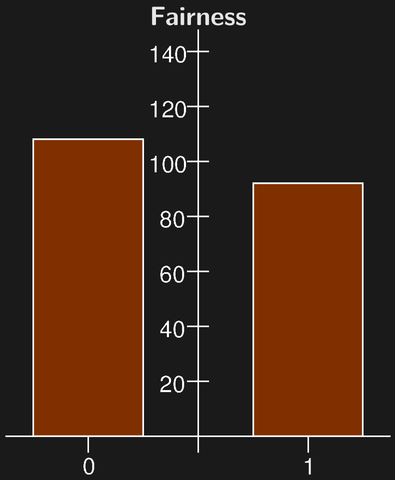
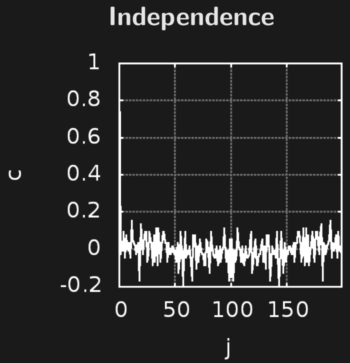
Test C++11 way, N=200



Fair



Uncorrelated

Other tests

- Moments
- Spacings between random points should follow a Poisson integral if uniformly distributed.
- Examine sequences of 5 numbers. There are 120 ways to sort 5 numbers. The 120 ways should occur with equal probability.
- Parking circle test: randomly place unit circles in a 100 x 100 square. If the circle overlaps an existing one, try again. After 12,000 tries, the number of successfully "parked" circles should follow a certain normal distribution.
- Play 200,000 games of a dice game (e.g. craps), counting the wins and number of throws per game. Each count follow a certain distribution.
- And many others. See, for example, the NIST test suite: http://csrc.nist.gov/groups/ST/toolkit/rng.

Good and Bad PRNGs

Some good PRNGs

- r1279 (good lagged-Fibonacci generator).
- Mersenne twister (mt19937).
- WELL generator (Well Equidistributed Long-period Linear, developed at U. Montréal).

Some not-so-good PRNGs:

- r250 (bad lagged-Fibonacci generator).
- Anything from Numerical Recipes - short periods, slow, ran0 and ran1
- spectacularly fail statistical tests.
- Standard Unix generators, rand(), drand48() - short periods, correlations.

Monte Carlo

Monte Carlo Techniques

A collection of techniques whose unifying feature is the use of randomness. These applications of randomness generally fall into one of three categories:

- Adding randomness to otherwise-deterministic dynamics, and studying how the dynamics are changed.
- Generating samples from a given probability distribution, $P(x)$, usually a distribution that is complicated and can't be dealt with nicely in closed form (e.g. Markov Chain Monte Carlo).
- Estimating expectation values under this distribution, e.g.

$$\langle A(\mathbf{x}) \rangle = \int P(\mathbf{x}) A(\mathbf{x}) d\mathbf{x}$$

  where $\mathbf{x}$ is typically high dimensional.

These depend on having a good random number generator!

MC example: traffic flow

Nagel-Schreckenberg traffic is a 1D toy model used to generate traffic-like behaviour. At each time step in the model, the following rules are applied to each car in the simulation:

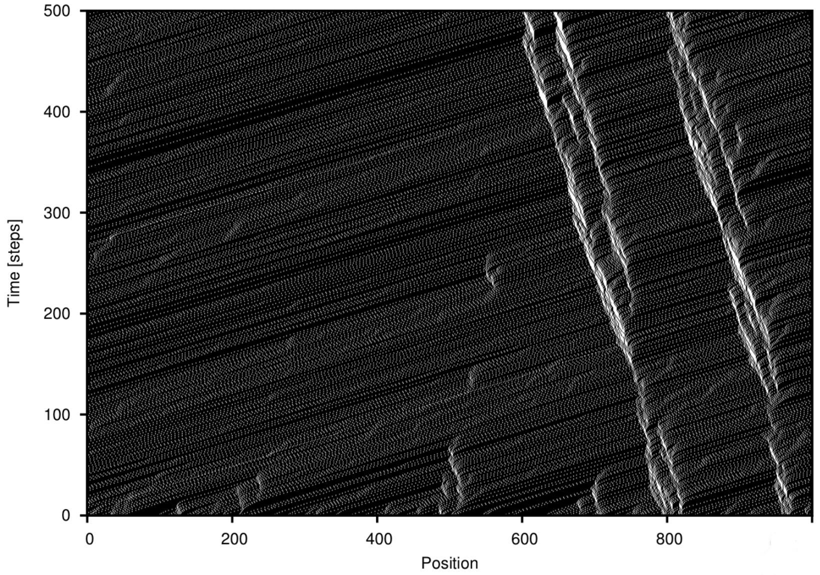
1. If the velocity is below vmax, then increase v by 1 (try to speed up).
2. If the car in front of the given car is a distance d away, and v$\geq$d, then reduce v to d-1 (don't want to hit the car).
3. Add randomness: if v>0 then with probability p the car reduces its speed by 1.
4. The car moves ahead by v steps (on a circular track).

The four rules boil down to

$$
\begin{aligned}
v &\leftarrow \min(v+1, v_{max}) \\
v &\leftarrow \min(v, d-1) \\
v &\leftarrow v-1 \text{ if } v \neq 0 \text{ with probability } p \\
x &\leftarrow x+v
\end{aligned}
$$

Monte Carlo example: traffic flow

numcars=200
gridsize=1000
p=0.13
vmax=5



Intermezzo

$$v \leftarrow v - 1 \text{ if } v \neq 0 \text{ with probability } p$$

How do you do that?

Intermezzo

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How do you do that?

- Draw a random number r using a PRNG with uniform distribution on $[0, 1)$.
- For any chosen value $p \in [0, 1)$, the chance that r is less than that value, is p itself.
- So if r is less than p, we will accept the move and decrease v if possible.
- If r is greater than or equal to p, we leave v as it is, i.e., we reject the move.

Monte Carlo Example: Molecular Motion

Consider a simple molecular dynamics model, which consists of a collection of molecules. For each timestep:

1. Randomly perturb the position of a given molecule.
2. Calculate the new total energy of the system, e.g., by a sum over pairwise potentials.
   - If the energy of the system goes down, keep the new position.
   - If the energy of the system goes up, keep the position if $r < \exp(-\Delta E/T)$, where r is a random number between 0 and 1, and T is the system temperature.
3. Repeat for all molecules.
4. Repeat for all timesteps.

Note: This is meant for sampling, it is not the real dynamics of molecules!

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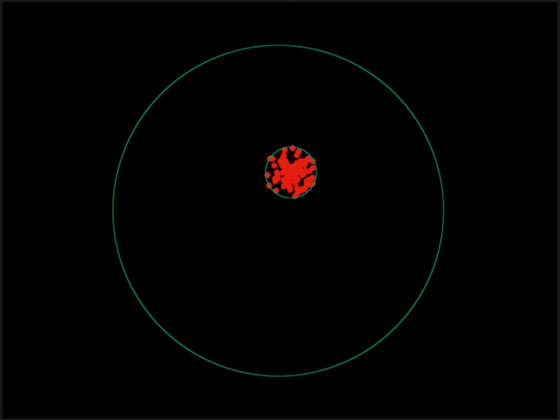

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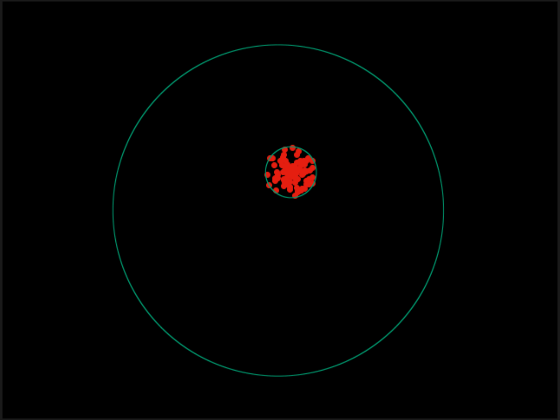

t=1000